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(54) Title: CRYSTAL STRUCTURE OF A DEACETYLASE AND INHIBITORS THEREOF

(57) Abstract: The present invention provides three-dimensional structural information from the hyperthermophilic bacterium *Aquifex aeolicus* which is a histone deacetylase-like protein (HDLP). HDLP shares 35.2% amino acid sequence identity with human histone deacetylase (HDAC1). The present invention further provides three-dimensional structural information of HDLP bound by inhibitor molecules. The three-dimensional structural information of the present invention is useful to design, isolate and screen deacetylase inhibitor compounds capable of inhibiting HDLP, HDAC family members and HDLP-related molecules. The invention also relates to nucleic acids encoding a mutant HDLP which facilitates the determination of the three-dimensional structure of HDLP in the presence of a zinc atom.

Crystal Structure of a Deacetylase and Inhibitors Thereof

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This application claims priority of U.S. Provisional Application No. 60/152,753, filed September 8, 1999, the contents of which are hereby incorporated by reference.

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This invention has been made with government support under National Institutes of Health Grant No. RO1 CA-65698. Accordingly, the U.S. Government may have certain rights in the invention.

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Throughout this application, various publications are referenced by author, date and citation. The disclosures of these publications in their entireties are hereby incorporated by reference into this application in order to more fully describe the state of the art as known to those skilled therein as of the date of the invention described and claimed herein.

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Introduction

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The present invention relates to a histone deacetylase homologue from the hyperthermophilic bacterium *Aquifex aeolicus*, HDLP (histone deacetylase like protein; also known as AcuCl), which shares 35.2 % sequence identity with human histone deacetylase (HDAC1), that can be co-crystallized with an inhibitory ligand, and more particularly, to the detailed crystallographic data obtained from said co-crystallization which is disclosed herein. The invention also relates to methods of using the crystal structure and x-ray crystallographic coordinates of the apo-HDLP and

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inhibitor-bound HDLP to design, isolate and screen compounds which bind to and inhibit the active site of HDLP and HDLP-related proteins, such as those proteins belonging to the HDAC family, including HDAC1.

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Background of the Invention

The reversible modification of histones by acetylation is associated with changes in nucleosome conformation and chromatin structure, and plays an important role in the regulation of gene expression (reviewed in Davie and Chadee, 10 1998, *J. Cell Biochem. Suppl.* 30-31:203-213). The histone acetylase and deacetylase enzymes that carry out these modifications are involved in many cellular processes such as cell cycle progression and differentiation, and their 15 deregulation is associated with several types of human cancer (reviewed in Kouzarides, 1999, *Curr. Opin. Genet. Dev.* 9:40-48; Hassig et al., 1997, *Chem. Biol.* 4:783-789; Fenrick and Heibert, 1998, *J. Cell. Biochem. Suppl.* 30-31:194-202).

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Recently, several experimental antitumor compounds, such as trichostatin A (TSA), trapoxin, suberoylanilide hydroxamic acid (SAHA), and phenylbutyrate have been shown to act, at least in part, by inhibiting histone deacetylases. Richon et 25 al., 1998, *Proc. Natl. Acad. Sci., USA* 95:3003-3007; Yoshida et al., 1990, *J. Biol. Chem.* 265:17174-17179; Kijima et al., 1993, *J. Biol. Chem.* 268:22429-22435. Additionally, diallyl sulfide and related molecules (Lea et al., 1999, *Int. J. Oncol.* 2:347-352), oxamflatin (Kim et al., 1999, *Oncogene* 30 15:2461-2470), MS-27-275, a synthetic benzamide derivative (Saito et al., 1999, *Proc. Natl. Acad. Sci.* 96:4592-4597),

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butarate derivatives (Lea and Tulsyan, 1995, *Anticancer Res.* 15:879-883), FR901228 (Nokajima et al., 1998, *Exp. Cell Res.* 241:126-133), depudecin (Kwon et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:3356-3361) and m-carboxysinnamic acid
5 bishydroxamide (CBHA; Richon et al., *Proc. Natl. Acad. Sci. USA* 95:3003-3007) have been shown to inhibit histone deacetylases. In vitro, these compounds can inhibit the growth of fibroblast cells by causing cell cycle arrest in the G1 and G2 phases (Richon et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:5705-5708; Kim et al., 1999, *Oncogene* 18:2461-2470; Yoshida et al., 1995, *Bioessays* 17:423-430; Yoshida & Beppu, 1988, *Exp. Cell. Res.* 177:122-131), and can lead to the terminal differentiation and loss of transforming potential of a variety of transformed cell
10 lines. Richon et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:5705-5708; Kim et al., 1999, *Oncogene* 18:2461-2470; Yoshida et al., 1987, *Cancer Res.* 47:3688-3691. In vivo, phenylbutyrate is effective in the treatment of acute promyelocytic leukemia in conjunction with retinoic acid.
15 Warrell et al., 1998, *J. Natl. Cancer Inst.* 90:1621-1625. SAHA is effective in preventing the formation of mammary tumors in rats, and lung tumors in mice. Desai et al., 1999, *Proc. AACR* 40: abstract #2396; Cohen et al., *Cancer Res.*, submitted.

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Histone deacetylases catalyze the removal of acetyl groups from the ϵ -amino groups of lysine residues clustered near the N-terminus of nucleosomal histones, and this process is associated with transcriptional repression (reviewed in
30 Struhl, 1998, *Genes Dev.* 12:599-606). Deletion of the yeast histone deacetylase gene, *rpd3*, or its pharmacological

inactivation with trichostatin A reduces the transcriptional repression in a subset of promoters, such as those of Ume6-regulated genes. Kadosh & Struhl, 1998, *Mol. Cell. Biol.* 18:5121-5127. This is accompanied by the increased
5 acetylation of H4 histones in the repressed promoter and its vicinity, but has no effect on histones at promoter distal regions. Kadosh & Struhl, 1998, *Mol. Cell. Biol.* 18:5121-5127; Rundlett et al., 1998, *Nature* 392:831-835.

10 Histone deacetylases are recruited to specific promoters by associating with DNA-binding transcriptional repressors, either directly or through co-repressors that bridge the deacetylase to the transcriptional repressors. For example, the Mad and Ume6 repressors bind to the co-repressor Sin3A
15 (Laherty et al., 1997, *Cell* 89:349-356; Hassig et al., 1997, *Cell* 89:341-347; Kadosh & Struhl, 1997, *Cell* 89:365-371), and the nuclear receptors bind N-CoR and the related SMRT co-repressors. Nagy et al., 1997, *Cell* 89:373-380; Alland et al, 1997, *Nature* 387:49-55; Heinzl et al, 1997, *Nature*
20 387:43-48.

The deregulation of histone deacetylase recruitment appears to be one of the mechanisms through which these enzymes contribute to tumorigenesis. In acute promyelocytic
25 leukemia (APL), chromosomal translocations fuse the retinoic acid receptor- α (RAR α) to either PLZF or to PML. These fusion oncoproteins have aberrant transcriptional repression activity resulting, in part, through the recruitment of a co-repressor and, in turn, HDACs. Grignani et al, 1998,
30 *Nature* 391:815-818; Lin et al., 1998, *Nature* 391:811-814. Treatment of PLZF-RAR α APL cells with TSA enhances their

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responsiveness to retinoic acid-induced differentiation. Grignani et al, 1998, *Nature* 391:815-818; Lin et al., 1998, *Nature* 391:811-814.

5 The histone deacetylases comprise a large family of proteins, conserved from yeast to man, and are divided into two related classes. Class I is characterized by human HDAC1, 2, 3 (Taunton et al., 1996, *Science* 272:408-411; Yang et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:12845-12850; 10 Emiliani et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:2795-2800), and yeast RPD3 (Videl & Gaber, 1991, *Mol. Cell. Biol.* 11:6317-6327), and class II by the human HDAC4, 5, 6 (Grozinger et al., 1999, *Proc. Natl. Acad. Sci. USA* 96:4868-4873; Fischle, et al., 1999, *J. Biol. Chem.* 274:11713-15 11720), and yeast HDA1 (Rundlett et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:14503-14508). The two classes share a ~390 amino acid region of sequence similarity, comprising the deacetylase core, but are divergent outside this region. The histone deacetylase genes belong to an even larger 20 superfamily (Leipe & Landsman, 1997, *Nucleic Acids Res.* 25:3693-3697) that contains the prokaryotic acetoin utilization proteins (AcuC; 28.1% sequence identity to HDAC1), and the prokaryotic acetylpolymine amidohydrolases (APAH; 15.0 % sequence identity to HDAC1). The enzymatic 25 activity of AcuC is not clear, but its disruption reduces the ability of *B. subtilis* to breakdown acetoin and utilize it as a carbon source. Grundy et al., 1993, *Mol. Microbiol.* 10:259-271. APAHs catalyze the deacetylation of polyamines by cleaving a non-peptide amide bond (reviewed in Leipe & 30 Landsman, 1997, *Nucleic Acids Res.* 25:3693-3697).

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It is useful to address the questions of how HDACs and HDAC-related proteins catalyze the deacetylation of histones and how the above-referenced compounds, particularly those compounds with antitumor activity, inhibit this activity in order to better understand the mechanism of inhibition of HDACs and to facilitate discovery of additional useful compounds which may inhibit this activity. To this end, the present invention has determined the three dimensional structure of a HDAC1-like protein from the thermophilic bacterium *Aquifex aeolicus*, herein after HDLP. The determination of the nucleic acid coding sequence of HDLP was described by Deckert et al., 1998, *Nature* 392:353-358. The encoded 375 residue protein, whose sequence was determined from the nucleic acid encoding sequence, shares 35.2% amino acid sequence identity with HDAC1, deacetylates histones *in vitro*, and is inhibited by TSA, SAHA and several other HDAC inhibitors. The determination of the three-dimensional structure of HDLP is useful in the design, identification and screening of new HDAC family inhibitory compounds which are useful for the inhibition of cell growth both *in vivo* and *in vitro*.

Summary of the Invention

In general, it is the object of the present invention to provide detailed three-dimensional structural information for a family of proteins known as histone deacetylases (HDAC), and particularly a homologue from the hyperthermophilic bacterium *Aquifex aeolicus* HDLP (histone deacetylase-like protein) which shares 35.2 % sequence identity with human histone deacetylase (HDAC1). It is also an object of the present invention to provide three-

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dimensional structural information of an HDLP bound to an inhibitory compound.

5 In one embodiment of the invention, three-dimensional structure information is obtained from a crystal of wild-type HDLP (SEQ ID NO:1) (the nucleic acid encoding wild-type HDLP is SEQ ID NO:2). In a further embodiment of the invention, three-dimensional information is obtained from a mutant HDLP comprising two mutations (1) cysteine 75 to a
10 serine and (2) cysteine 77 to a serine (Cys75Ser/Cys77Ser double mutant; SEQ ID NO:3) (the nucleic acid encoding HDLP Cys75Ser/Cys77Ser double mutant is SEQ ID NO:4). The HDLP mutant of the present invention facilitates the determination of three-dimensional structural information of
15 HDLP bound to a zinc atom at its zinc atom-binding site.

In a preferred embodiment of the invention, the three-dimensional structural information is obtained from a co-crystal of a protein-inhibitor compound complex that
20 comprises HDLP or HDLP Cys75Ser/Cys77Ser double mutant and trichostatin A (TSA). In another preferred embodiment of the invention the three-dimensional structural information is obtained from a co-crystal of a protein-inhibitor compound complex that comprises HDLP or HDLP
25 Cys75Ser/Cys77Ser double mutant and suberoylanilide hydroxamic acid (SAHA). Any HDLP or HDLP-related protein (e.g. HDAC) inhibitor compound that may be co-crystallized with HDLP may be used to form a co-crystal of the present invention.

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The protein crystals and protein-inhibitory complex co-crystals of the present invention diffract to a high

resolution limit of at least equal to or greater than 4 angstrom (Å). In a preferred embodiment, the protein crystals and protein-inhibitory complex co-crystals of the present invention diffract to a high resolution limit of
5 greater than 2.5 Å.

A crystal of the present invention may take a variety of forms, all of which are contemplated by the present invention. In a preferred embodiment, the crystal has a
10 space group of C2 with one molecule in the asymmetric unit and with unit dimensions of $a = 51.4 \text{ Å}$, $b = 93.8 \text{ Å}$, $c = 78.7 \text{ Å}$ and $\beta = 96.9^\circ$ (see, e.g., Example 2, below). In another preferred embodiment, the crystal has a space group of $P2_12_12_1$ with two molecules in the asymmetric unit and with
15 unit dimensions of $a = 53.4 \text{ Å}$, $b = 94.4 \text{ Å}$, $c = 156.3 \text{ Å}$ (see, e.g., Example 2, below). The HDLP structure comprises a parallel β sheet with α helices packing against both faces. At one end of the β sheet, the HDLP has a narrow, tube-like pocket formed by several well-ordered loops. The walls of
20 the pocket are lined with hydrophobic residues and there is a zinc binding site and several polar side chains at the bottom of the pocket. The inhibitory compounds of the present invention bind in the pocket.

25 The three-dimensional structural information obtained from crystals of HDLP, HDLP Cys75Ser/Cys77Ser double mutant, HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc atom, HDLP comprising an inhibitory compound such as TSA or SAHA, and HDLP Cys75Ser/Cys77Ser double mutant comprising an inhibitor
30 compound such as TSA or SAHA may be employed to solve the structure of any HDLP-related protein (e.g. HDAC) crystal,

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or any mutant HDLP-related protein and particularly any wild type or mutant of HDLP-related protein complexed with a ligand, including a substrate or inhibitor compound. If the crystals are in a different space group than the known structure, molecular replacement may be employed to solve the structure, or if the crystals are in the same space group, refinement and difference fourier methods may be employed. The structure of HDLP-related proteins (e.g. HDAC1) comprise no greater than a 2.0 Å root mean square deviation (rmsd) in the positions of the C α atoms for at least 50% or more of the amino acids of the full-length HDLP structure.

The present invention also provides a nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant having the amino acid sequence of SEQ ID NO:3 and the nucleic acid sequence of SEQ ID NO:4. It is also contemplated by the invention that mutations be made in HDLP-related proteins at cysteine residues, as with the Cys75Ser/Cys77Ser double mutant, in order to facilitate the determination of the structure of said proteins bound to a zinc atom. Additionally, the present invention provides expression vectors which comprise the nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant encoded by the sequence represented by SEQ ID NO:4 operatively linked to expression control sequences.

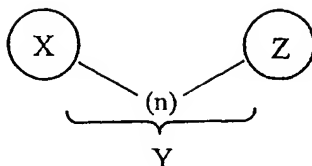
It is another object of the present invention to provide methods for the design, identification and screening of potential inhibitor compounds of the HDLP/HDAC family. In a preferred embodiment the method for the rational design,

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identification and screening of potential inhibitor compounds for HDLP and HDLP-related proteins (e.g. HDACs) comprising deacetylase activity comprises the steps of: (a) using a three-dimensional structure of an HDLP as defined by the atomic coordinates of the present invention; (b) employing said three-dimensional structure to design or select said potential inhibitor compound; (c) synthesizing and/or selecting said potential inhibitor; (d) contacting said potential inhibitor compound with said enzyme in the presence of acetylated substrate; and (e) determining the percent inhibition of deacetylase activity to determine the inhibitory activity of said potential inhibitor compound. In a further preferred embodiment, the binding properties of said rationally designed inhibitory compound may be determined by a method comprising the steps of: (a) forming a complex comprising said inhibitory compound and HDLP or a HDLP-related protein, (b) co-crystallizing said inhibitory compound-HDLP complex; (c) determining said three-dimensional structure of said co-crystal through molecular replacement or refinement and difference fourier with the molecular coordinates of HDLP as defined by the present invention; and (d) analyzing the three-dimensional structure to determine the binding characteristics of said potential inhibitor compound.

It is a further object of the present invention to identify a defined class of HDLP/HDAC family inhibitor compounds. The HDLP/HDAC family inhibitor compounds of the present invention are represented by formula (I):

(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises an active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and may further bind to a zinc atom.

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Brief Description of the Drawings

Figure 1 is a table listing the statistics from the X-ray crystallographic analysis of a HDLP crystal, a HDLP-TSA co-crystal, and a HDLP-SAHA co-crystal.

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Figure 2 shows an alignment of various HDAC homologues with percent sequence identity depicted.

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Figure 3 shows a graph indicating the histone deacetylase activity of HDLP and HDAC1 and the inhibition of HDLP and HDAC1 by the inhibitors TSA and HC-toxin.

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Figure 4 shows (A & B) a schematic representation of the HDLP-Zn²⁺-TSA complex in two approximately orthogonal views, (C) a topology diagram of HDLP indicating the regions of homology with HDAC1, and (D) a close-up schematic representation of the HDLP-Zn²⁺-SAHA complex.

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Figure 5 shows (A) a schematic representation of a slice through a surface representation of HDLP with the pocket internal cavities and position of the β sheet indicated, (B) a schematic representation of a close-up view of the active site looking down into the pocket in an orientation similar to Figure 4B.

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Figure 6 shows (A) a space-filling representation of TSA in the active site pocket, (B) a closeup stereo view of the structure of the HDLP-ZN²⁺-TSA complex in a similar orientation to Figure 4B, and (C) a schematic representation of the HDLP-TSA interactions.

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Figure 7 shows (A) a schematic representation of the regions of homology shared between HDLP and HDAC1 in an orientation similar to that of Figure 4A, and (B) a detailed schematic representation of the homology shared in the pocket and
5 internal cavity between HDLP and HDAC1 in an orientation similar to that of Figure 4B.

Figure 8 shows a schematic representation of the proposed catalytic mechanism for the deacetylation of acetylated
10 lysine.

Figure 9 shows a schematic representation of a space filling diagram showing the conserved amino acids in the active site and nearby grooves.
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Figure 10 is the nucleic acid sequence of HDLP from *Aquifex aeolicus* (SEQ ID NO. 2).

Figure 11 is the amino acid sequence of full length HDLP
20 from *Aquifex aeolicus* (SEQ ID NO. 1).

Figure 12 is the nucleic acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 6).

25 Figure 13 is the amino acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 5).

Figure 14 is the nucleic acid sequence of a double mutant of HDLP from *Aquifex aeolicus* comprising a Cys75Ser and
30 Cys77Ser mutation (SEQ ID NO. 4).

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Figure 15 is the amino acid sequence of a double mutant of HDLP from *Aquifex aeolicus* comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 3).

5 Figure 16-1 to 16-49 lists the atomic structure coordinates for HDLP as derived by X-ray diffraction from a crystal of HDLP.

10 Figure 17-1 to 17-49 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc atom in the active site as derived by X-ray diffraction from a crystal of the HDLP Cys75Ser/Cys77Ser double mutant.

15 Figure 18-1 to 18-99 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray diffraction from a co-crystal of HDLP complexed with TSA.

20 Figure 19-1 to 19-48 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray diffraction from a co-crystal of HDLP complexed with SAHA.

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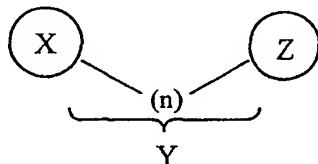
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Detailed Description of the Invention

The present invention provides crystals of a histone deacetylase (HDAC) homologue grown in the presence and absence of a compound capable of inhibiting the histone deacetylase activity of said HDAC homologue. As referred to herein, a HDAC homologue (as well as a HDLP-related protein) is any protein molecule having (a) greater than 15% sequence identity to over the 375 amino acid residues of HDLP; (b) having no more than twenty insertions or deletions for a total of no more than 100 amino acids; and (c) deacetylase activity. Sequence identity is calculated by the program DNASTar™ using the identity matrix weighing scheme clustal method (DNASTar program, Madison, WI).

A HDLP/HDAC inhibitor compound, as used herein, refers to any compound represented by Formula (I):

(I)



wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of tyrosine, proline and leucine; Y comprises an aliphatic chain group from about 5 to about 10 Å, preferably 7 Å, which binds to at least one amino acid selected from the group consisting of phenylalanine and glycine; and Z comprises a active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and which may further bind to a zinc atom. The HDAC inhibitory compounds of the present

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invention can inhibit greater than 50% of the histone deacetylase activity of a HDAC homologue or a HDLP-related protein.

5 To grow the crystals of the present invention, the HDAC and HDAC-inhibitory compound complex are purified to greater than 80% total protein and more preferably purified to greater than 90% total protein. For expression and purification purposes, the full-length HDLP (Genbank
10 accession number AE000719) may be subcloned from *Aquifex aeolicus* chromosomal DNA preparation by the polymerase chain reaction (PCR) and inserted into an expression vector.

A large number of vector-host systems known in the art may
15 be used. Possible vectors include, but are not limited to, plasmids or modified viruses, but the vector system must be compatible with the host cell used. Examples of vectors include *E. coli* bacteriophages such as lambda derivatives, or plasmids such as pBR322 derivatives or pUC plasmid
20 derivatives, e.g., pGEX vectors (Amersham-Pharmacia, Piscataway, New Jersey), pET vectors (Novagen, Madison, WI), pmal-c vectors (Amersham-Pharmacia, Piscataway, New Jersey), pFLAG vectors (Chiang and Roeder, 1993, *Pept. Res.* 6:62-64), baculovirus vectors (Invitrogen, Carlsbad, CA; Pharmingen,
25 San Diego, CA), etc. The insertion into a cloning vector can, for example, be accomplished by ligating the DNA fragment into a cloning vector which has complementary cohesive termini, by blunt end ligation if no complementary cohesive termini are available or by through nucleotide
30 linkers using techniques standard in the art. E.g., Ausubel et al. (eds.), *Current Protocols in Molecular*

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Biology, (1992). Recombinant vectors comprising the nucleic acid of interest may then be introduced into a host cell compatible with the vector (e.g. *E. coli*, insect cells, mammalian cells, etc.) via transformation, transfection, 5 infection, electroporation, etc. The nucleic acid may also be placed in a shuttle vector which may be cloned and propagated to large quantities in bacteria and then introduced into a eukaryotic cell host for expression. The vector systems of the present invention may provide 10 expression control sequences and may allow for the expression of proteins *in vitro*.

In a preferred embodiment, the full length HDLP (SEQ ID NO:2) is subcloned from *Aquifex aeolicus* chromosomal DNA 15 preparation into pGEX4T3 (Amersham-Pharmacia, Piscataway, New Jersey). In order to construct a double mutant comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO:4), and to construct the HDLP active site mutant Tyr297Phe (SEQ ID NO:5 and SEQ ID NO:6), PCR site directed mutagenesis may 20 be employed with verification by DNA sequencing by methods known to those skilled in the art (see, e.g., Example 1 below). The mutants of the present invention may be subcloned into a suitable expression vector and introduced into a host cell for protein production, as described above.

25 The HDLP nucleic acids of the present invention may be subcloned into an expression vector to create an expression construct such that the resultant HDLP molecule which is produced comprises a fusion protein wherein said fusion 30 protein comprises a tag for ease of purification. As referred to herein, a "tag" is any additional amino acids

which are provided in a protein either c-terminally, n-terminally or internally for the ease of purification, for the improvement of production or for any other purpose which may facilitate the goals of the present invention (e.g. to achieve higher levels of production and/or purification). Such tags include tags known to those skilled in the art to be useful in purification such as, but not limited to, his tag, glutathione-s-transferase tag, flag tag, mbp (maltose binding protein) tag, etc. In a preferred embodiment, the wild-type and mutant HDLPs of the present invention are tagged with glutathione-s-transferase (see Example 1 below). In another preferred embodiment, HDAC1 is flag tagged (see Example 1 below). Such tagged proteins may also be engineered to comprise a cleavage site, such as a thrombin, enterokinase or factor X cleavage site, for ease of removal of the tag before, during or after purification. Vector systems which provide a tag and a cleavage site for removal of the tag are particularly useful to make the expression constructs of the present invention.

The tagged HDLPs and HDACs of the present invention may be purified by immuno-affinity or conventional chromatography, including but not limited to, chromatography employing the following: glutathione-sepharose™ (Amersham-Pharmacia, Piscataway, New Jersey) or an equivalent resin, nickel or cobalt-purification resins, anion exchange chromatography, cation exchange chromatography, hydrophobic resins, gel filtration, antFLAG epitope resin, reverse phase chromatography, etc. After purification, the HDLP and HDLP-inhibitor compound complex may be concentrated to greater than 1 mg/ml for crystallization purposes. In a preferred embodiment HDLP and HDLP-inhibitor complexes are

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concentrated to greater than 10 mg/ml for crystallization and in a particularly preferred embodiment, HDLP and HDLP-inhibitor complexes are concentrated to greater than 20 mg/ml.

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In order to determine whether the purified HDLPs of the present invention demonstrate histone deacetylase activity, the purified HDLPs and also any HDLP-related protein may be assayed by any method known to those skilled in the art for the determination of said activity. In a preferred embodiment, the purified HDLPs of the present invention are incubated in the presence of [³H]acetyl-labeled histone substrate (Carmen et al., 1996, *J. Biol. Chem.* 271:15837-15844) in a buffer suitable for detection of histone deacetylase activity (see Example 3 below); stopping the reaction; extracting the released acetate and measuring said released acetate, as described by Henzel et al. (*J. Biol. Chem.* 266:21936-21942 (1991); Example 3 below). In a preferred embodiment, the HDLPs of the present invention are incubated in the presence of ZnCl₂ in order to obtain histone deacetylase activity therefrom (Example 3 below).

In another embodiment, the crystals of the present invention comprise purified wild-type HDLP (SEQ ID NO:1) and are grown at room temperature by the hanging-drop vapor-diffusion method from a crystallization solution comprising one or more precipitants selected from the group consisting of isopropanol, polyethylene glycol, and tert butanol (see Example 2 below). The crystallization solution may further comprise one or more salts including salts selected from the group consisting of NaCl and KCl, and one or more buffers

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including buffers selected from the group consisting of Tris (tris(hydroxymethyl)aminomethane and bis-tris propane-Cl (1,3-bis[tris(hydroxymethyl)methyl-amino] propane) (see Example 2 below). The pH of the crystallization solution is preferably between pH 5 to 9, although other pH values are also contemplated by the present invention (see Example 2 below).

Any crystallization technique known to those skilled in the art may be employed to obtain the crystals of the present invention, including, but not limited to, batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and micro dialysis. Seeding of the crystals in some instances may be required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used.

The crystals of the present invention may form in the space group C2 with one molecule in the asymmetric unit and with unit dimensions of $a = 51.4 \text{ \AA}$, $b = 93.8 \text{ \AA}$, $c = 78.7 \text{ \AA}$ and $\beta = 96.9^\circ$ (see Example 2 below). The crystals of the present invention may also form in the space group $P2_12_12_1$ with two molecules in the asymmetric unit and with unit dimensions of $a = 53.4 \text{ \AA}$, $b = 94.4 \text{ \AA}$, $c = 156.3 \text{ \AA}$ (see Example 2 below). However, the present invention contemplates crystals which form in any space group including, but not limited to, C2, $P2_1$, $P2_12_12_1$, $P3_12_1$, $P4_32_12_1$, and C222₁. The crystals diffract to a resolution greater than 4 \AA , preferably greater than 2.5 \AA .

To collect diffraction data from the crystals of the present

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invention, the crystals may be flash-frozen in the crystallization buffer employed for the growth of said crystals, however with preferably higher precipitant concentration (see, e.g., Example 2 below). For example, but not by way of limitation, if the precipitant used was 28% PEG 1500, the crystals may be flash frozen in the same crystallization solution employed for said crystal growth wherein the concentration of the precipitant is increased to 35% (see Example 2 below). If the precipitant is not a sufficient cryoprotectant (*i.e.* a glass is not formed upon flash-freezing), cryoprotectants (*e.g.* glycerol, low molecular weight PEGs, alcohols, etc) may be added to the solution in order to achieve glass formation upon flash-freezing, providing the cryoprotectant is compatible with preserving the integrity of the crystals. The flash-frozen crystals are maintained at a temperature of less than -110°C and preferably less than -150°C during the collection of the crystallographic data by X-ray diffraction. The X-ray diffraction data may be processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, *Method Ensemble*. 276:307-326) but any method known to those skilled in the art may be used to process the X-ray diffraction data.

In order to determine the atomic structure of HDLP according to the present invention, multiple isomorphous replacement (MIR) analysis, model building and refinement may be performed. For MIR analysis, the crystals may be soaked in heavy-atoms to produce heavy atom derivatives necessary for MIR analysis. As used herein, heavy atom derivative or derivitization refers to the method of producing a chemically modified form of a protein or protein complex

crystal wherein said protein is specifically bound to a heavy atom within the crystal. In practice a crystal is soaked in a solution containing heavy metal atoms or salts, or organometallic compounds, e.g., lead chloride, gold cyanide, thimerosal, lead acetate, uranyl acetate, mercury chloride, gold chloride, etc, which can diffuse through the crystal and bind specifically to the protein. The location(s) of the bound heavy metal atom(s) or salts can be determined by X-ray diffraction analysis of the soaked crystal. This information is used to generate MIR phase information which is used to construct the three-dimensional structure of the crystallized HDLPs and HDLP-related proteins of the present invention. In a preferred embodiment, the heavy atoms comprise thimerosal, $\text{KAu}(\text{CN})_2$ and $\text{Pb}(\text{Me})_3\text{OAc}$ (see Example 2 below). The MIR phases may be calculated by any program known to those skilled in the art and preferably with the program MLPHARE (The CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D.* 50:760-763) and may also use the anomalous diffraction signal from the thimerosal derivative. In a preferred embodiment, the MIR phases were calculated at 2.5 Å and have a mean figure of merit of 0.55 (see Figure 19 and Example 2 below). The phases may be improved where necessary by solvent flattening by methods known to those skilled in the art including, but not limited to, through the use of the program DM (The CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D* 50:760-763).

Thereafter, an initial model of the three-dimensional structure may be built using the program O (Jones et al.,

1991, *Acta Crystallogr. A* 47:110-119). The interpretation and building of the structure may be further facilitated by use of the program CNS (Brunger et al., 1998, *Acta Crystallogr. D* 54:905-921).

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For the determination of the HDLP-inhibitor compound complex structure, if the space group of the HDLP-inhibitor compound complex crystal is different, molecular replacement may be employed using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure whose structure may be determined as described above and below in Example 2. If the space group of the HDLP-inhibitor compound crystals is the same, then rigid body refinement and difference fourier may be employed to solve the structure using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure.

20

The term "molecular replacement" refers to a method that involves generating a preliminary model of the three-dimensional structure of the HDLP crystals of the present invention whose structure coordinates are unknown prior to the employment of molecular replacement. Molecular replacement is achieved by orienting and positioning a molecule whose structure coordinates are known (in this case the previously determined apo-HDLP) within the unit cell as defined by the X-ray diffraction pattern obtained from an HDLP or HDLP-related protein crystal whose structure is

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unknown so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of several forms of refinement to provide a final, accurate structure.

Any method known to the skilled artisan may be employed to determine the structure by molecular replacement. For example, the program AMORE (The CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D.* 50:760-763) may be employed to determine the structure of an unknown histone deacetylase +/- an inhibitor by molecular replacement using the apo-HDLF coordinates (Figure 16). For the structure determination of the inhibitory compound TSA, the structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST, << <http://www.ccdc.cam.ac.uk> >>) may be employed to define the stereochemical restraints used in the refinement with the program CNS (Brunger et al., 1998, *Acta Crystallogr. D* 54:905-921).

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP are useful for solving the structure of crystallized proteins which belong to the HDAC family by molecular replacement. Similarly, any structure of a crystallized protein which is thought to be similar in structure based on function or sequence similarity or identity to HDLP may be solved by molecular replacement with the HDLP structural

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information of the present invention. The structure of HDLP-related proteins as determined by molecular replacement as described above and in Example 2 below, comprise a root mean square deviation (rmsd) of no greater than 2.0 Å in the positions of Cα atoms for at least 50% or more of the amino acids of the structure over the 375 residues of full-length HDLP. Such a rmsd may be expected based on the amino acid sequence identity. Chothia & Lesk, 1986, *Embo J.* 5:823-826.

The refined three-dimensional HDLP structures of the present invention, specifically apo-HDLP, Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site, HDLP/TSA complex comprising a zinc atom in the active site, and HDLP/SAHA complex comprising a zinc atom in the active site, are represented by the atomic coordinates set forth in Figures 16 to 19 respectively. The refined model for apo-HDLP comprising amino acids 1-375 consists of wild-type HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution of 1.8 Å. Similarly, the refined model for Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site also consists of residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution of 2.0 Å. The refined model for the HDLP/TSA complex comprising a zinc atom in the active site consists of the Cys75Ser/Cys77Ser double mutant HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered, has TSA in the binding pocket and was determined to a resolution of 2.1 Å. The HDLP/SAHA complex is similar to the HDLP/TSA complex but has SAHA in the binding pocket and was determined to a resolution of 2.5 Å.

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For the purposes of further describing the structure of HDLP and HDLP-related proteins, including, but not limited to, HDACs, from the data obtained from the HDLP crystals of the present invention, the definition of the following terms is provided:

The term " β sheet" refers to two or more polypeptide chains (or β strands) that run alongside each other and are linked in a regular manner by hydrogen bonds between the main chain C=O and N-H groups. Therefore all hydrogen bonds in a beta-sheet are between different segments of polypeptide. Most β -sheets in proteins are all-parallel (protein interiors) or all-antiparallel (one side facing solvent, the other facing the hydrophobic core). Hydrogen bonds in antiparallel sheets are perpendicular to the chain direction and spaced evenly as pairs between strands. Hydrogen bonds in parallel sheets are slanted with respect to the chain direction and spaced evenly between strands.

The term " α helix" refers to the most abundant helical conformation found in globular proteins. The average length of an α helix is 10 residues. In an α helix, all amide protons point toward the N-terminus and all carbonyl oxygens point toward the C-terminus. The repeating nature of the phi, psi pairs ensure this orientation. Hydrogen bonds within an α helix also display a repeating pattern in which the backbone C=O of residue X (wherein X refers to any amino acid) hydrogen bonds to the backbone HN of residue X+4. The α helix is a coiled structure characterized by 3.6 residues per turn, and translating along its axis 1.5 Å per amino acid. Thus the pitch is 3.6x1.5 or 5.4 Å. The screw sense of alpha helices is always right-handed.

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The term "loop" refers to any other conformation of amino acids (i.e. not a helix, strand or sheet). Additionally, a loop may contain bond interactions between amino acid side chains, but not in a repetitive, regular fashion.

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Amino acid residues in peptides shall herein after be abbreviated as follows: Phenylalanine is Phe or F; Leucine is Leu or L; Isoleucine is Ile or I; Methionine is Met or M; Valine is Val or V; Serine is Ser or S; Proline is Pro or P; Threonine is Thr or T; Alanine is Ala or A; Tyrosine is Tyr or Y; Histidine is His or H; Glutamine is Gln or Q; Asparagine is Asn or N; Lysine is Lys or K; Aspartic Acid is Asp or D; Glutamic Acid is Glu or E; Cysteine is Cys or C; Tryptophan is Trp or W; Arginine is Arg or R; and Glycine is Gly or G. For further description of amino acids, please refer to *Proteins: Structure and Molecular Properties* by Creighton, T.E., W.H. Freeman & Co., New York 1983.

The term "positively charged amino acid" refers to any amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged amino acids are Arg, Lys and His. The term "negatively charged amino acid" refers to any amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged amino acids are Asp and Glu. The term "hydrophobic amino acid" refers to any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of hydrophobic amino acids are Ala, Leu, Ile, Gly, Val, Pro, Phe, Trp and Met. The term "hydrophilic amino acid" refers to any amino acid having an uncharged, polar side chain that is

relatively soluble in water. Examples of hydrophilic amino acids are Ser, Thr, Tyr, Asp, Gln, and Cys. The term "aromatic amino acid" refers to any amino acid comprising a ring structure. Examples of aromatic amino acids are His, Phe, Trp and Tyr.

The term "charge relay system" refers to a His-Asp arrangement as described by Fersht & Sperling, 1973, *J. Mol. Biol.* 74:137-149; Blow et al., 1969, *Nature* 221:337-340.

The information obtained from the three-dimensional structures of the present invention reveal that HDLP has a single-domain structure that belongs to the open α/β class of folds (see, e.g., Branden, 1980, *Q. Rev. Biophys.* 13:317-38). Two orthogonal views of the overall three-dimensional structure of HDLP are depicted in Figure 4A and 4B. The HDLP structure has a central eight-stranded parallel β sheet (strands arranged as $\beta 2$ - $\beta 1$ - $\beta 3$ - $\beta 8$ - $\beta 7$ - $\beta 4$ - $\beta 5$ - $\beta 6$), and sixteen α helices (labeled $\alpha 1$ through $\alpha 16$ respectively). See Figure 4C. Four of the helices pack on either face of the β sheet ($\alpha 7$, $\alpha 8$, $\alpha 9$, $\alpha 10$ and $\alpha 11$, $\alpha 12$, $\alpha 13$, $\alpha 14$) forming the core α/β structure characteristic of this class of folds. Most of the remaining eight helices are positioned near one side of the β sheet, near strands $\beta 2$ - $\beta 1$ - $\beta 3$ - $\beta 8$. Large, well defined loops (Loops L1-L7; Figure 4C) originate from the C-terminal ends of the β -strands. The extra helices and the large L1-L7 loops are associated with a significant extension of the structure beyond the core α/β motif. This extension of the structure gives rise to two prominent architectural features: a deep, narrow pocket and an internal cavity adjacent to the pocket. These

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two architectural features comprise the active site (see Figure 5A). The structure of HDLP-related proteins (e.g. HDACs) may also comprise the conserved α/β structure characteristic.

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The term "active site" comprises any or all of the following sites in HDLP, the substrate binding site, the site where the cleavage of an acetyl group from a substrate occurs or the site where an inhibitor of the HDAC family or, more particularly, HDLP binds. The active site, as referred to
10 herein, comprises Asp166, Asp258, His170, Tyr297, His131, His132, Asp168, Asp173, Phe141, Phe198, Leu265, Pro22 and Gly140, and also a metal bound at the bottom of the pocket by Asp173, Asp168 and His defined by the coordinates listed
15 in Figures 16 to 19 with an rmsd of 2.0 Å. The metal which binds at the bottom of the pocket will be a divalent cation selected from the group consisting of zinc, cobalt or manganese.

20 The deep narrow pocket has a tube-like shape with a depth of ~ 11 Å. The pocket opening constricts half way down to ~ 4.5 by 5.5 Å, and becomes wider at the bottom (see Figure 5A). The pocket and its immediate surroundings are made up of loops L1 through L7.

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The walls of the pocket are covered with side chains of hydrophobic and aromatic residues (Pro22, Tyr91 near the entrance; and Gly140, Phe141, Phe 198, Leu265 and Tyr297 further down; Figure 5B). For numbering of amino acids
30 please refer to SEQ ID NO:1. Of particular interest are Phe141 and Phe198, whose phenyl groups face each other in

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parallel at a distance of 7.5 Å, marking the most slender portion of the pocket (see Figure 5B). Of particular interest is that only one pocket residue differs in HDAC1 when the sequences are aligned (alignment may be accomplished using DNASTar™ MegAlign™ program, Madison, WI), this residue is Glu98 of HDAC1 which is Tyr91 in HDLP. The structure reveals that this residue in HDLP is mostly solvent exposed.

10 Near the bottom of the pocket of the active site at its narrowest point, is located a zinc ion (see Figure 6A). In order to obtain the zinc in the structure, the crystals may be soaked in zinc (e.g. ZnCl₂) or co-crystallized in the presence of zinc. The zinc ion is coordinated by Asp168 (Oδ1, 2.1 Å), His170 (Nδ1, 2.1 Å), Asp258 (Oδ1, 1.9 Å) and a water molecule (2.5 Å). See Figure 5B and 6B. The amino acid residues that coordinate zinc are arranged in a tetrahedral geometry, but the position of the water molecule, which is also hydrogen bonded to His131, deviates from this geometry by ~25°.

In addition to the zinc ligands, the bottom of the pocket contains two histidine (His131 and His132), two aspartic acids (Asp166 and Asp173) and a tyrosine (Tyr297). See Figure 5B and 10B. Each of the histidines makes a hydrogen bond through its Nδ1 to an aspartic acid carboxylate oxygen, with the oxygen located in the plane of the imidazole ring (Figure 5B). This His-Asp arrangement is characteristic of the charge relay system present in the active sites of serine proteases, where it serves to polarize the imidazole Ne and increase its basicity. Fersht & Sperling, 1973, J.

Mol. Biol. 74:137-149; Blow et al., 1969, *Nature* 221:337-340.

5 The Asp166-His131 charge pair relay (hereafter referred to as "buried charged relay") is positioned even deeper in the pocket and more buried compared to the Asp173-His132 charge relay (hereafter referred to as "exposed charge relay") which is partially solvent exposed. The buried charge relay makes a hydrogen bond (2.6 Å) to the zinc-bound water
10 molecule referred to above, and this hydrogen bond could contribute to the deviation of the water-zinc coordination from ideal geometry (Figure 5B). The exposed charge relay is directed to a point ~ 2.5 Å away from the water molecule and closer to the surface.

15 Tyr 297 is positioned next to the zinc, opposite from where the two charge relay systems are located. The Tyr hydroxyl group lies 4.4 Å away from the zinc atom and has no interactions with the rest of the protein (Figure 5B). Next
20 to Tyr297, there is an opening in the pocket wall, which leads to the adjacent internal cavity.

The floor of the internal cavity is made up of portions of the L3 and L7 loops as they emerge from the β strands, and
25 the roof is made up by the α1-L1-α2 segment. The L1 loop appears more flexible than other loops in the structure. This may allow the transient exchange of the cavity contents with the bulk solvent.

30 The cavity is lined primarily with hydrophobic residues and is particularly rich in glycine residues (Ala127, Gly128, Gly129, Met130, and Phe141 of L3; Gly293, Gly294, Gly295 and

Gly296 of L7; and Tyr17, Pro22 and Leu23 of L1). There are only two charged residues in the cavity (Arg27 and His 21) and these are contributed by the L1 loop.

5 The cavity may provide space for the diffusion of the acetate product away from the catalytic center, which may otherwise be crowded and shielded during deacetylation from the solvent when the substrate is bound. Such a role for the cavity is supported by the observation that the cavity
10 contains three water and two isopropanol molecules (from the crystallization buffer) in the 1.8 Å apo-protein structure. The cavity may also bind another cofactor, in addition to zinc, for the facilitation of the enzymatic activity of the HDLP. A proposed catalytic mechanism for deacetylation is
15 provided in Figure 8.

The structure of HDLP as defined by the present invention, in conjunction with the HDAC1 sequence homology, shows that the 375-amino acid HDLP protein corresponds to the histone
20 deacetylase catalytic core which is conserved across the HDAC family (see Figure 2). The 35.2% HDLP-HDAC1 sequence identity predicts structural similarity with a rmsd in C α positions of ~ 1.5 Å. Chothia and Lesk describe the relation between the divergence of sequence and the
25 structure of proteins in *Embo J.* 5:823-826 (1986). The 40-residue C-terminus of HDLP is likely to have a divergent structure since this region has lower homology to HDAC1, although the α 16 helix in this region is part of the conserved open α/β core fold and HDAC1 is likely to comprise
30 a similar helix. However divergent this C-terminal region may be, this region is outside the active site and is likely to not effect the structure of the active site. Beyond the

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C-terminus of the histone deacetylase catalytic core, HDAC family members are divergent in length and sequence. In the HDAC family, this region (amino acid residues ~390-482) is highly polar, populated with acidic residues, and is likely to be flexible or loosely folded.

The HDLP-HDAC homology maps primarily to the hydrophobic core and to the L1-L7 loops, with portions of the loops that make up the pocket and adjacent cavity having the highest level of amino acid residue sequence conservation (Figure 9A and 9B). Specifically, all of the polar residues in the active site (the zinc ligands, the two charge relay systems, and Tyr297) and the hydrophobic residues that make up the walls of the pocket (Gly140, Phe141, Phe198 and Leu265) are identical. Among the residues that make up the internal cavity, the ones closest to the active site are either identical or conservatively substituted (for example, Leu23 → Met and Met130 → Leu). Surface residues around the pocket are conserved to a lesser extent, but are still above 35% average sequence identity.

The information obtained from the inhibitor-bound HDLP complex crystal structures of the present invention reveal detailed information which is useful in the design, isolation, screening and determination of potential inhibitor compounds which may inhibit HDLP/HDAC family members. As described above, the HDLP structure consists of a parallel β sheet with α helices packing against both faces (Figure 4A, 4B, and 4C). At one end of the β sheet, 7 loops (L1-L7) form a narrow, tube-like pocket which are lined with hydrophobic residues and which comprise a zinc binding site, several polar side chains, including two Asp-His charge

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relay systems. Mutation of the zinc ligands and other polar residues at the pocket bottom reduces or eliminates the catalytic activity.

5 The present inventors found that mutation at the Tyr297Phe site reduced activity. See also, Hassig et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:3519-3524; Kadosh & Struhl, 1998, *Genes Dev.* 12:797-805. The elimination of activity by
10 mutation of these residues indicates that this region is the enzyme active site. Adjacent to the active site, there is an internal cavity that may provide space for the diffusion of the acetate reaction product. Homology at the active site between HDLP and HDAC1, as described above, indicates that they share structural and functional homology.

15 The inhibitor compound, trichostatin A (TSA) (Tsuji et al., 1976, *J. Antibiotics* 29:1-6) binds HDLP by inserting its long aliphatic chain, which has a hydroxamic acid group at one end, into the pocket (Figure 6A, 6B and 6C). The
20 aliphatic chain makes multiple contacts in the well-like, hydrophobic portion of the pocket. The hydroxamic acid reaches the polar bottom of the pocket, where it coordinates the zinc in a bidentate fashion and also forms hydrogen bonds with the polar residues in the active site, including
25 the two charge relay system histidines. The aromatic dimethylamino-phenyl group at the other end of the TSA chain makes contacts at the pocket entrance and serves to cap it. The amino acid residues of HDLP which contact TSA are conserved in HDAC, indicating that TSA binds and inhibits
30 HDAC in a similar fashion to HDLP.

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In the complex, the hydroxamic acid, most of the aliphatic chain and part of the dimethylamino-phenyl group of TSA are buried (60% of TSA's surface area; Figure 6A). The hydroxamic acid group binds the zinc in a bidentate fashion forming bonds through its carbonyl (2.4 Å) and hydroxyl groups (2.2 Å) resulting in a penta-coordinated Zn^{2+} (Figure 6B and 6C). The hydroxamic acid hydroxyl group replaces the water molecule that binds to the zinc in the apo-HDLP structure described above. The hydroxamic acid also hydrogen bonds with both charge relay system histidines (hydroxyl oxygen to His131 Ne2, 2.8 Å; and nitrogen to His132 Ne2, 2.8 Å), and the Tyr297 hydroxyl group (2.4 Å; Figure 6B and 6C).

The 5-carbon long branched alkene chain of TSA fits snugly in the narrow portion of the pocket making multiple van der Waals contacts with all of the hydrophobic groups lining the pocket (Figure 6B and 6C). Near its center, the chain contains a methyl substituted carbon-carbon double bond which is sandwiched between the phenyl groups of the Phe141 and Phe98 at the tightest point of the pocket (Figure 6A and 6B). The length of the alkene chain appears optimal for spanning the length of the pocket, and allowing contacts both at the bottom and at the entrance of the pocket, although, the cap group of Formula (I) may provide length to span the pocket allowing for a shorter alkene chain (aliphatic chain).

At the entrance of the pocket, one face of the planar structure formed by the dimethylamino-phenyl and adjacent carbonyl groups of TSA makes contacts at the rim of the pocket (Pro22, Tyr91, Phe141; Figure 6B and 6C). This

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packing is facilitated by the roughly 110° angle in the overall structure of TSA at the junction of the aliphatic chain and the dimethylamino-phenyl group (occurring at the sp³ hybridized C8 carbon). Upon TSA binding, the side chain of Tyr91, which is mostly solvent exposed, changes conformation to make space for the dimethylamino-phenyl group. This is the only change near the active site observed upon TSA binding.

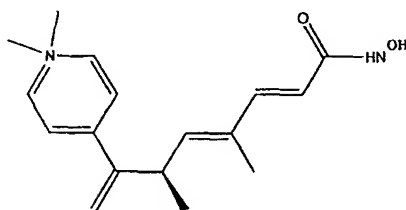
The hydroxamic acid group is a common motif in zinc metalloprotease inhibitors. See U.S. Patent No. 5,919,940 and 5,917,090; See also, Grams et al., 1995, *Biochemistry* 34:14012-14020; Lovejoy et al., 1999, *Nat. Struct. Biol.* 6:217-221; and Holmes & Matthews, 1981, *Biochemistry* 20:6912-6920. Like TSA, these inhibitors also coordinate the active site zinc in a bidentate fashion using their hydroxamate hydroxyl and carbonyl oxygens, replace the nucleophilic water molecule with their hydroxamate hydroxyl groups and form hydrogen bonds to the general base (Grams et al., 1995, *Biochemistry* 34:14012-14020; Lovejoy et al., 1999, *Nat. Struct. Biol.* 6:217-221; and Holmes & Matthews, 1981, *Biochemistry* 20:6912-6920).

SAHA, which has a ~30-fold weaker inhibitory activity than TSA (Richon et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:3003-3007), binds HDLP similarly to TSA (see, e.g., Figure 4D). The SAHA hydroxamic acid group makes the same contacts to the zinc and active site residues, and the importance of these interactions is underscored by the loss of activity of SAHA derivatives lacking the hydroxamic group (Richon et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:3003-

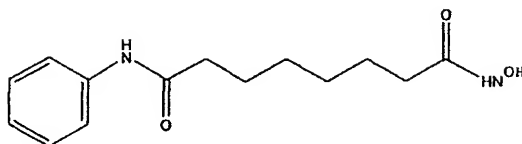
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3007). The six-carbon long aliphatic chain of SAHA packs in the tube-like hydrophobic portion of the pocket. Compared to TSA however, SAHA's aliphatic chain packs less snugly and makes fewer van der Waals contacts, in part, because SAHA lacks TSA's C15 methyl group branch. SAHA also lacks TSA's double bonds in this region, and this may lead to increased flexibility of the aliphatic chain. The cap group of SAHA consists of a phenyl-amino ketone group. In the crystal structure, the phenyl group has weak electron density, suggesting that it does not pack as well as the cap group of TSA. This may be due to the larger separation between the hydroxamic and cap groups of SAHA compared to TSA (compare TSA, Formula (II) and SAHA, Formula (III), below).

(II)



(III)

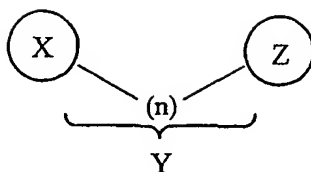


The determination of the structure of HDLP and HDLP bound to an inhibitory compound has enabled, for the first time, the identification of the active site of HDLP and of related HDLP proteins, such as proteins belonging to the HDAC family.

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP bound to an inhibitory compound is useful in rational drug design providing for a method of identifying inhibitory compounds which bind to and inhibit the enzymatic activity of HDLP, HDAC family proteins and other histone deacetylase-like proteins related to HDLP. Said method for identifying said potential inhibitor for an enzyme comprising deacetylase activity comprises the steps of (a) using a three-dimensional structure of HDLP as defined by its atomic coordinates listed in Figure 16 to 19; (b) employing said three-dimensional structure to design or select said potential inhibitor; (c) synthesizing said potential inhibitor; (d) contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and (e) determining the ability of said inhibitor to inhibit said deacetylase activity.

The potential HDLP and HDLP-related (e.g. HDAC) inhibitors identified by the method of the present invention are represented by formula (I)

(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises an active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and wherein Z may further bind to a zinc atom and with the provision that the compound of Formula (I) is not TSA, trapoxin, SAHA, SAHA derivatives described in U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5840,960 and 5,668,179.

The present invention permits the use of molecular design techniques to design, identify and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site of HDLP and HDLP-related proteins. The atomic coordinates of apo-HDLP and inhibitor-bound HDLP may be used in conjunction with computer modeling using a docking program such as GRAM, DOCK, HOOK or AUTODOCK (Dunbrack et al., 1997, *Folding & Design* 2:27-42) to identify potential inhibitors of HDLP and HDLP-related proteins (e.g. HDAC1). This procedure can include computer fitting of potential inhibitors to the active site of HDLP to ascertain how well the shape and the

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- 40 -

chemical structure of the potential inhibitor will complement the active site or to compare the potential inhibitors with the binding of TSA or SAHA in the active site. See Bugg et al, 1998, *Scientific American* December:92-98; West et al., 1995, *TIPS* 16:67-74. The potential inhibitors designed by modeling with a docking program conform to the general formula (I) as described above. Computer programs may also be employed to estimate the attraction, repulsion and stearic hindrance of the HDLP and potential inhibitor compound. Generally, the tighter the fit, the lower the stearic hindrances, the greater the attractive forces, and the greater the specificity which are important features for a specific inhibitory compound which is more likely to interact with HDLP and HDLP-related proteins rather than other classes of proteins. These features are desired particularly where the inhibitory compound is a potential antitumor drug.

The compounds of the present invention may also be designed by visually inspecting the three-dimensional structure to determine more effective deacetylase inhibitors. This type of modeling may be referred to as "manual" drug design. Manual drug design may employ visual inspection and analysis using a graphics visualization program such as "O" (Jones, T.A., Zhou, J.Y., Cowan, S.W., and Kjeldgaard, M., Improved method for building protein models in electron density maps and the location of errors in these models, *Acta Crystallog.*, A47, 110-119.

Initially potential inhibitor compounds can be selected for their structural similarity to the X, Y and Z constituents

of formula (I) by manual drug design. The structural analog thus designed can then be modified by computer modeling programs to better define the most likely effective candidates. Reduction of the number of potential candidates is useful as it may not be possible to synthesize and screen a countless number of variations compounds that may have some similarity to known inhibitory molecules. Such analysis has been shown effective in the development of HIV protease inhibitors (Lam et al., 1994, *Science* 263:380-384; Wlodawer et al., 1993, *Ann. Rev. Biochem.* 62:543-585; Appelt, 1993 *Perspectives in Drug Discovery and Design* 1:23-48; Erickson, 1993, *Perspectives in Drug Discovery and Design* 1:109-128. Alternatively, random screening of an small molecule library could lead to potential inhibitors whose inhibitory activity may then be analyzed by computer modeling as described above to better determine their effectiveness as inhibitors.

The compounds designed using the information of the present invention may be competitive or noncompetitive inhibitors. These designed inhibitors may bind to all or a portion of the active site of HDLP and may be more potent, more specific, less toxic and more effective than known inhibitors for HDLP and HDLP-related proteins, and particularly HDACs. The designed inhibitors may also be less potent but have a longer half life *in vivo* and/or *in vitro* and therefore be more effective at inhibiting histone deacetylase activity *in vivo* and/or *in vivo* for prolonged periods of time. Said designed inhibitors are useful to inhibit the histone deacetylase activity of HDLP and HDLP-related proteins (e.g. HDAC1), to inhibit cell growth in

vitro and in vivo and may be particularly useful as antitumor agents.

5 The present invention also permits the use of molecular design techniques to computationally screen small molecule data bases for chemical entities or compounds that can bind to HDLP in a manner analogous to the TSA and SAHA as defined by the structure of the present invention. Such computational screening may identify various groups which
10 may be defined as "X", "Y" or "Z" of formula (I) above and may be employed to synthesize the potential inhibitors of the present invention comprising formula (I). Such potential inhibitors may be assayed for histone deacetylase inhibitory activity in a histone deacetylase activity assay
15 (see Example 3 below), may be co-crystallized with HDLP to determine the binding characteristics through X-ray crystallography techniques defined above (e.g. said co-crystal structure may be determined by molecular replacement to assess the binding characteristics of said potential
20 inhibitor), or may be assessed based on binding activity by incubating said potential inhibitor with said HDLP, performing gel filtration to separate any free potential inhibitor to HDLP-bound inhibitor, and determining the amount of histone deacetylase activity of the inhibitor-bound HDLP. To measure binding constants (e.g., K_d),
25 methods known to those in the art may be employed such as Biacore™ analysis, isothermal titration calorimetry, Elisa with a known drug on the plate to show competitive binding, or by a deacetylase activity assay.

The design of potential inhibitors of the present invention is further facilitated by reference to Figure 9, which is a surface representation figure that depicts the surface grooves. Analysis of such grooves gives insight into the constituents of the cap group of formula (I). The surface grooves are labeled groove A, groove A', groove B and groove C, into which additional cap groups may bind. The structure of HDLP bound to either TSA or SAHA shows that the cap groups of TSA and SAHA bind in groove A. By analysis of the amino acid sequence identity of HDLP and HDACs, Groove A is well conserved in HDACs, has a significant hydrophobic component, appears deep enough to allow for significant interactions and is also the largest of the four grooves. In addition to the dimethylamino phenyl group of the TSA, the A groove can fit approximately 200 daltons worth of groups (e.g. groove A could accommodate a naphthalene-like group after an appropriate spacer, etc.). Groove A, as referred to herein, is characterized by the following conserved residues of HDLP: His 21, Pro22, Lys24, Phe141, Leu265 and Phe335. The periphery of groove A comprises unconserved residues. Additionally, Groove A', as referred to herein, comprises primarily unconserved residues.

Groove B is immediately adjacent to the pocket. Of significance is that the bottom of groove B comprises the N-epsilon nitrogen of His170, which coordinates the zinc through its N-delta nitrogen. Significant binding energy may be achieved by contacting the Ne proton of His170 with a carboxylic acid or sulfate group. In addition, groove B may be large enough to fit a phenyl group, the face of which may comprise a partial negative charge which may pack over the N-epsilon proton of His170. The conserved residues of

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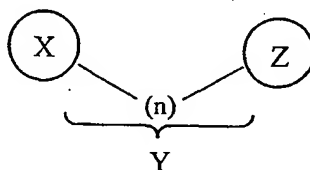
groove B, as referred to herein are: His170, Tyr196 and Leu265.

5 Groove C is not as well conserved as the other two grooves and the amino acid residues which comprise groove C are mostly polar and solvent exposed. Groove C, as referred to herein comprises the following conserved residues: Asn87, Gly140 and Phe198.

10 The compounds of the present invention are represented by formula (I):

(I)

15

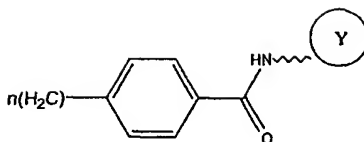


20 Examples for suitable X constituents wherein X comprises a cap group may be described in three categories, depending upon which surface of groove A, A', B and/or C they are targeted to. The cap group may comprise all three categories on the same compound. Of particular benefit may be replacing the cap group of TSA or SAHA with a large, rigid structure. Nonlimiting examples for suitable cap groups (X) of formula (I) which may bind in groove A are:

25 (1) attaching a 1-3 methyl linker followed by a phenyl or naphthalene group from the para or meta position of SAHA's phenyl group represented by formula (IV):

30

(IV)

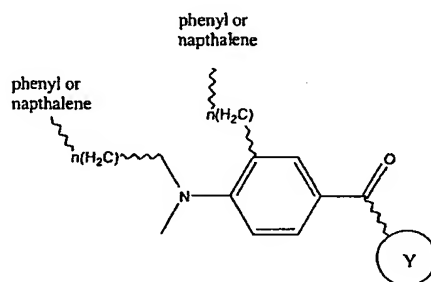


5

(2) attaching a 2-3 methyl linker followed by a phenyl or naphthalene group from the meta position of TSA's phenyl cap group, or from TSA's dimethyl amino group represented by formula (V):

10

(V)

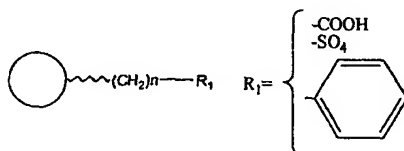


15

and which may bind in groove B is a 1-3 methyl group spacer followed by a carboxylate, sulfate or phenyl group as represented by formula (VI):

20

(VI)



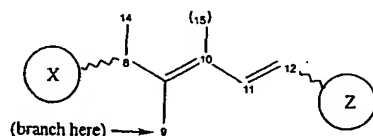
25

With respect to the aliphatic (Y) group, the diameter of the pocket suggests that one more methyl "side chain" could fit, in addition to the C15 methyl group on the C10 carbon. Nonlimiting suitable examples for Y constituents wherein Y comprises an aliphatic chain group are as follows: (1) add

30

a methyl group to TSA on the C12 carbon (with or without a methyl group on the C10 carbon and with or without double bonds and with or without substituting the X and/or Z constituents of formula (I) as represented by formula (VII):

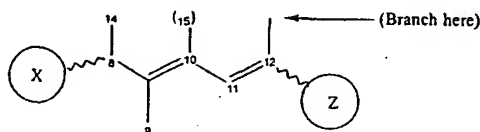
5 (VII)



10 (2) add a methyl group to TSA on the C9 carbon (with or without a methyl group on the C10 carbon; with or without both or either of the double bonds, and with or without substituting the X and/or Z constituents of formula (I) as represented by formula (VIII):

15

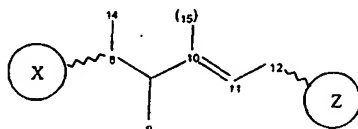
(VIII)



20

(3) replace the two alkalene double bonds of TSA with only one between C10 and C11, which may free the C11 and C12 torsion to allow for a better fit, the X and/or Z groups may also be substituted as represented by formula (IX):

25 (IX)



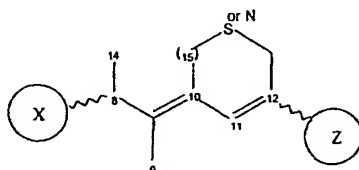
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(4) cyclize C15 and C12 carbons of TSA through a sulphur atom (or nitrogen atom), the X and/or Z groups may also be substituted as represented by formula (X):

(X)

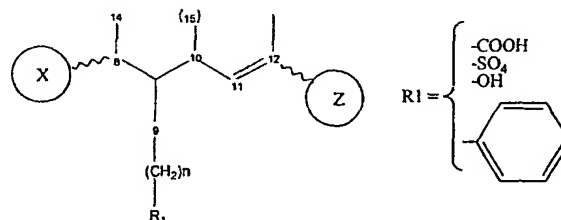
5



(5) extend from the C9 carbon of TSA such that the extension approaches and/or enters groove B (see Figure 9); making C9 sp³ so that it can have some freedom; attach to C9 a 1-3 methyl group spacer which may include a double bond and they attaching thereto a sulfate, carboxylate, sulfate, hydroxyl, or phenyl group which may make an interaction with the N-epsilon proton of His170 which may coordinate the zinc atom as represented by formula (XI):

(XI)

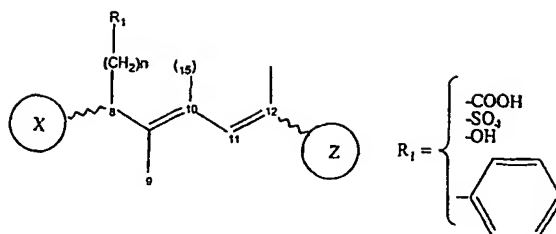
20



(6) extend off the C8 carbon (replacing C14) of TSA such that the extension approaches or enters groove B; attach a 1-3 methyl group spacer (which may include a double bond) and then link thereto a carboxylate, sulfate, hydroxyl or phenyl group such that an interaction is made with the N-epsilon proton of His170 that coordinates the zinc atom; the X and/or Z constituents may also be substituted as represented by formula (XII):

(XII)

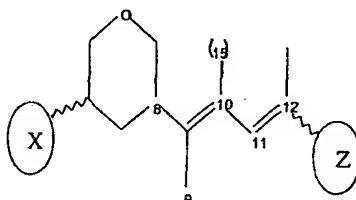
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(7) substitute the C8 carbon at the end of the aliphatic chain such that the substitution may contact groove A, A', B and or C, in such an example, a cap group (X) may or may not be required and the X and Z constituents may be substituted as well, as represented by formula (XIII):

(XIII)

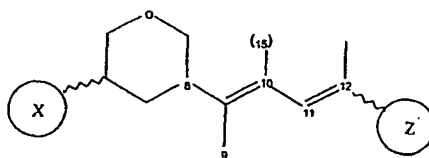
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(8) formulas VII through XIII above wherein the aliphatic chain further comprises a methyl group between the active site binding group (Z) and the C8 carbon, and preferably just before the C8 carbon, increasing the distance between X and Z, (9) make the connection between the aliphatic chain and the cap group more rigid (e.g., by closing a 6-membered ring which may or may not comprise oxygen, the X and Z group may also be substituted as represented by formula (XIV):

(XIV)

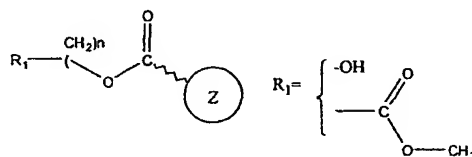
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and (10) combining two or more of the changes depicted by formulas (VII-XIV).

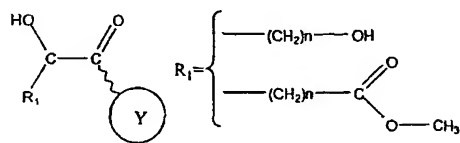
Additionally, nonlimiting examples for suitable Z groups wherein Z comprises an active site binding group are as follows: (1) hydroxamic acid, (2) carboxylic acid, (3) sulfonamide, (4) acetamide, (5) epoxyketone, (6) an ester with a methyl linker and a hydroxyl of acetate ester group to lead into the cavity and interact with a conserved arginine (Arg27) as represented by formula (XV):

(XV)



and (7) an alphaketone as represented by formula (XVI):

(XVI)



Additionally, other suitable X, Y and Z constituents may be envisioned by the skilled artisan given the three-dimensional structural information of the present invention.

After having determined potential suitable X, Y and Z constituents, the constituents are combined to form a compound of formula (I) using combinatorial chemistry techniques. This may be achieved according to U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5,840,960 and 5,668,179, incorporated herein by reference. Any methods

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known to one of skill in the art may be employed to synthesize compounds of formula (I) comprising X, Y and Z constituents as determined by the methods described above.

5 As mentioned above, the compounds of formula (I) are useful to inhibit the histone deacetylase activity of HDLP and HDAC-related proteins. Such inhibition may allow for a reduction or cessation of cell growth *in vitro* and *in vivo*.

10 For *in vitro* use, such reduction or cessation of cell growth is useful to study the role of histone deacetylation and differentiation during the cell cycle and also to study other mechanisms associated with cell cycle arrest and particularly how the repression of transcription is involved
15 in cell cycle progression which may be studied in a yeast model system such as that described by Kadosh & Struhl, 1998, *Mol. Cell. Biol.* 18:5121-5127. *In vitro* model systems which may be employed to study the effects of potential inhibitors on cell cycle progression and also tumor growth
20 include those described by: Richon et al, 1998, *Proc. Natl. Acad. Sci. USA* 95:3003-3007; Yoshida et al., 1995, *Bioessays* 17:423-430; Kim et al., 1999, *Oncogene* 18:2461-2470; Richon et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:5705-5708; and Yoshida et al., 1987, *Cancer Res.* 47:3688-3691.

25 For *in vivo* use, such a reduction or cessation of cell growth is useful to study the effect of said inhibitor compounds in non-human animal model systems of cancer and is also useful for the treatment of cancer in a recipient in
30 need of such treatment. Non-limiting examples of animals which may serve as non-human animal model systems include

mice, rats, rabbits, chickens, sheep, goats, cows, pigs, and non-human primates. See, e.g., Desai et al., 1999, *Proc. AACR 40*: abstract #2396; Cohen et al., 1999, *Cancer Res.*, submitted. The compounds of the present invention may be administered to a transgenic non-human animal wherein said animal has developed cancer such as those animal models in which the animal has a propensity for developing cancer (e.g. animal model systems described in U.S. Patents 5,777,193, 5,811,634, 5,709,844, 5,698,764, and 5,550,316). Such animal model systems may allow for the determination of toxicity and tumor reduction effectiveness of the compounds of the present invention.

A preferred compound of the present invention may comprise high specific activity for HDLP and HDAC-related proteins, good bioavailability when administered orally, activity in reducing or ceasing cell growth in tumor cell lines, and activity in reducing or ceasing tumor growth in animal models of various cancers.

Accordingly, another aspect of this invention is a method of eradicating or managing cancer in a recipient, which may be an animal and is preferably a human. Said method comprises administering to said recipient a tumor reducing amount of a compound as defined by formula (I) above, or a physiological acceptable salt thereof.

In a further aspect of the invention, there is provided a composition comprising the compound of formula (I) and an excipient or carrier. Administration of the foregoing agents may be local or systemic. Such carriers include any

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suitable physiological solutions or dispersant or the like. The physiologic solutions include any acceptable solution or dispersion media, such as saline, or buffered saline. The carrier may also include antibacterial and antifungal agents, isotonic and absorption delaying agents, and the like. Except insofar as any conventional media, carrier or agent is incompatible with the active ingredient, its use in the compositions is contemplated.

Routes of administration for the compositions containing the delivery vehicle constructs of the present invention include any conventional and physiologically acceptable routes, such as, for example, oral, pulmonary, parenteral (intramuscular, intraperitoneal, intravenous (IV) or subcutaneous injection), inhalation (via a fine powder formulation or a fine mist), transdermal, nasal, vaginal, rectal, or sublingual routes of administration and can be formulated in dosage forms appropriate for each route of administration.

The following examples are provided to more clearly illustrate the aspects of the invention and are not intended to limit the scope of the invention.

EXAMPLES

Example 1: Protein Production and Purification:

Full-length wild-type HDLP (Genbank accession number AE000719) was subcloned from an *Aquifex aeolicus* chromosomal DNA preparation (provided by Robert Huber of Universitaet of Regensburg, Germany) into the pGEX4T3 (Amersham-Pharmacia, Piscataway, NJ) vector using the polymerase chain reaction (PCR). The cysteine-to-serine and active site mutants were constructed by PCR site directed mutagenesis and were

sequenced. The HDLP-glutathione S-transferase (GST) fusion protein was produced in *Escherichia coli*, purified by affinity chromatography using a column of glutathione-sepharose resin (Amersham-Pharmacia, Piscataway, NJ), and by anion-exchange chromatography (Q-sepharose™; 5 Amersham-Pharmacia, Piscataway, NJ). HDLP was cleaved from the fusion protein with thrombin at 4° C, was purified by anion-exchange (Q-sepharose™; Amersham-Pharmacia, Piscataway, NJ) and gel filtration chromatography 10 (Superdex™200; Amersham-Pharmacia, Piscataway, NJ), and was concentrated to typically 25 mg/ml in a buffer of 25 mM bis-tris propane (BTP), 500 mM NaCl, 5 mM dithiothrietirol (DTT), 2% isopropanol, pH 7.0.

15 Although, it is not known what metal cofactor HDLP contains *in vivo*, it is presumed to be zinc because of the arrangement of the ligands and the similarities in the active site to the zinc proteases. The lack of metal in the purified HDLP is presumed due, in part, to the use of DTT 20 during purification. HDLP was reconstituted with Zn^{2+} by mixing the Cys75Ser/Cys77Ser double mutant at 10 mg/ml with a 5-fold molar excess of $ZnCl_2$ in a buffer of 25 mM bis-tris propane, 200 mM NaCl, 1% isopropanol, pH 7.0. Unbound $ZnCl_2$ was removed by fractionating HDLP through a G25 desalting 25 column (Amersham-Pharmacia, Piscataway, NJ). The HDLP- Zn^{2+} -TSA complex was prepared by incubating the Zn^{2+} reconstituted HDLP mutant with 1 mM TSA for 45 minutes, followed by gel filtration chromatography (Superdex™200; Amersham-Pharmacia, Piscataway, NJ) to remove excess TSA, 30 and concentration to typically 25 mg/ml in a buffer of 25 mM bis-tris propane, 500 mM NaCl, 1% isopropanol, pH 7.0.

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FLAG epitope tagged human HDAC1 was overexpressed using a baculovirus expression system in Hi5 (Invitrogen, Carlsbad, CA) insect cells grown in suspension in serum-free media (Sf900, Gibco, Grand Island, NY). The fusion protein was
5 purified by anion exchange and affinity chromatography using Anti-FLAG M2 affinity resin (Sigma, St. Louis, MO) and FLAG Peptide (Sigma,, St. Louis, MO).

Example 2: Crystallization and data collection:

10 Crystals of apo-HDLp were grown at room temperature by the hanging-drop vapor-diffusion method, from 7.5% isopropanol, 28% PEG 1500, 425 mM NaCl, 100 mM Tris-Cl, pH 7.0. They form in space group C2 with $a = 51.4 \text{ \AA}$, $b = 93.8 \text{ \AA}$, $c = 78.7 \text{ \AA}$, $\beta = 96.9 \text{ \AA}$, and contain one HDLP molecule in the
15 asymmetric unit. Diffraction data were collected with crystals flash-frozen in a buffer of 7.5% isopropanol, 35% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, at -170° C .

The structure of the HDLP- Zn^{2+} complex was determined from
20 HDLP Cys75Ser/Cys77Ser double mutant crystals grown from 23% tert-butanol, 27% PEG 1500, 400 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8. Space group and cell dimensions were identical to the apocrystals. The HDLP- Zn^{2+} crystals were harvested and frozen in 27% tert-butanol, 22% PEG 1500, 50
25 mM KCl, 20 mM NaCl, 0.2 mM ZnCl_2 , 100 mM bis-tris propane, pH 6.8, at -170° C .

Crystals of the HDLP- Zn^{2+} -TSA complex comprised HDLP Cys75Ser/Cys77Ser double mutant and were grown from 23%
30 tert-butanol, 27% PEG 1500, 600 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8, by microseeding. The crystals were grown in the presence of zinc. They form in space group

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P2₁2₁2₁ with $a = 53.4 \text{ \AA}$, $b = 94.4 \text{ \AA}$, $c = 156.3 \text{ \AA}$ and contain two HDLP- Zn²⁺-TSA complexes in the asymmetric unit. The HDLP-Zn²⁺-TSA crystals were harvested and frozen in the same cryobuffer as the HDLP- Zn²⁺ crystals except that 0.5mM TSA
5 was added. Data were processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, *Method. Ensemble.* 276:307-326). MIR analysis, model building and refinement.

The HDLP-Zn²⁺-SAHA complex crystals were grown and evaluated
10 the same as the HDLP-Zn²⁺-TSA crystals. However, the restraints for the SAHA structure were constructed based on stereochemical parameters from TSA. Like the apo-HDLP crystals, the SAHA/HDLP co-crystals grew in space group C2.

15 Heavy-atom soaks were performed with the apo-HDLP crystals in a buffer of 7.5% isopropanol, 30% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, supplemented with 1.0 mM thimerosal for 2h, 5 mM KAu(CN)₂ for 1h, and 1 mM Pb(Me)₃OAc for 2h. MIR phases were calculated with the program MLPHARE (The
20 CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D* 50:760-763) at 2.5 Å using the anomalous diffraction signal from the thimerosal derivative, and had a mean figure of merit of 0.55. The phases were improved by solvent flattening with the program DM (The CCP4
25 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D* 50:760-763) , and were used to build the initial model with the program O (Jones et al., 1991, *Acta Crystallogr. A* 47:110-109). Successive rounds of rebuilding and simulated annealing refinement with the
30 program CNS (Brunger et al., 1998, *Acta Crystallogr. D* 54:905-921) allowed interpretation of HDLP from residues 2

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to 373. Residues 1, 374, and 375 were not modeled and are presumed to be disordered.

5 The structure of the HDLP-Zn²⁺-TSA and HDLP-Zn²⁺-SAHA complex were determined by molecular replacement with the program AMORE (The CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D* 50:760-763) using the apo-HDLP structure as a search model. The initial electron density maps had strong and continuous difference
10 density for the entire TSA molecule. However the SAHA molecule was not as well ordered in the cap group region. The structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST) and was used to define stereochemical restraints used in the refinement with the
15 program CNS. The restraints of SAHA were constructed based on stereochemical parameters from TSA and surrounding amino acid residues. The dimer interface in the HDLP-Zn²⁺-TSA and HDLP-Zn²⁺-SAHA crystals primarily involves Phe200 on the protein surface. The Phe200 side chain contacts Tyr91,
20 whose side chain conformation changes on TSA binding, and part of the dimethyl amino phenyl group of TSA from the second protomer. The HDAC family does not contain a phenylalanine residue at the equivalent position.

25 Example 3: Histone deacetylase assays:

Purified proteins were assayed by incubating 10 µg of [3H]acetyl-labeled murine erythroleukemia histone substrate and HDAC assay buffer (20 mM Tris-HCl, pH 8.0, 150 mM NaCl, 10% glycerol) for 30-60 minutes at 37° C in a total volume
30 of 30 µl. The final concentrations of HDLP and HDAC1-FLAG were 3.6 µM and 0.24 µM, respectively. Assays were performed in duplicate. The reactions were stopped and the

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released acetate was extracted and assayed as described (Hendzel et al., 1991, *J. Biol. Chem.* 266:21936-21942). [3H]acetyl-labeled murine erythroleukemia histones were prepared essentially as described (Carmen et al., 1996, *J. Biol. Chem.* 271:15837-15844). Inhibitors were added in the
5 absence of substrate and incubated on ice for 20 minutes, substrate was added, and the assay performed as described above. HDLP was incubated with 20 μ M ZnCl₂ and 20 μ M MnCl₂(H₂O)₄ in HDAC buffer and tested for activity.

10

Only HDLP dialyzed against ZnCl₂ had activity. HDAC1-FLAG was dialyzed against 20 μ M ZnCl₂ in HDAC buffer which had no effect on activity. Therefore, HDAC1-FLAG contains a metal as purified.

15

The *in vivo* substrate of HDLP is not known. HDLP may have a role in acetoin utilization like the *B. subtilis* AcuC gene product, and it has been annotated as such in the genome sequence, but the reaction catalyzed by AcuC is also not
20 known. Furthermore, the *A. aeolicus* genome appears to lack the acuA and acuB genes that are part of the acuABC operon of *B. subtilis* (Deckert et al., 1998 *Nature* 392:353-358), and HDLP is as similar to human HDAC1 (35.2 % identity) as it is to *B. subtilis* AcuC (34.7 % identity).

25

What is claimed is:

1. A crystal of an enzyme comprising deacetylase activity wherein said crystal effectively diffracts X-rays for the determination of the atomic coordinates of said enzyme to a resolution of greater than 4 Å and wherein the structure of said enzyme comprises a conserved core α/β structure characteristic fold wherein said conserved α/β fold comprises an eight-stranded parallel β sheet and eight α helices and wherein four of the helices pack on either face of said parallel β sheet and wherein said structure of said enzyme comprises an rmsd of less than or equal to 1.5 Å in the positions of C α atoms for at least 2/3 or more of the amino acids of HDLP as defined by the atomic coordinates of HDLP.
2. The crystal of claim 1, wherein said protein structure further comprises:
 - (a) eight α helices positioned near one side of the β sheet; and
 - (b) at least seven large, well defined loops originating from the C-terminal ends of the β -strands of said eight-stranded parallel β sheet wherein the eight extra helices and the seven large loops are associated with a significant extension of the structure beyond the core α/β motif and wherein said extension of the structure gives rise to a deep, narrow pocket and an internal cavity adjacent to the pocket.
3. The crystal of claim 1, wherein said enzyme comprising deacetylase activity is selected from the group

consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, AcuC, and functional derivatives thereof.

5

4. The crystal of claim 2 further comprising a specifically bound zinc atom in the active site of said enzyme.

10

5. The crystal of claim 2 further comprising a specifically bound deacetylase inhibitor compound in the active site of said enzyme.

15

6. The crystal of claim 2 define by the atomic coordinates according to Figure 16.

20

7. A method for identifying a potential deacetylase inhibitor compound for an enzyme which comprises deacetylase activity, said method comprising the steps of:

25

- a. using a three-dimensional structure of HDLP as defined by atomic coordinates according to Figure 16;
- b. employing said three-dimensional structure to design or select said potential inhibitor;
- c. synthesizing said potential inhibitor;
- d. contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and

30

- e. determining the deacetylase inhibitory activity of said potential inhibitor.

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8. The method of claim 7, wherein the three-dimensional structure is designed or selected using computer modeling.
- 5 9. The method of claim 7, wherein the potential deacetylase inhibitor is designed de novo.
- 10 10. The method of claim 7, wherein the potential deacetylase inhibitor is designed based on a known inhibitor.
- 15 11. The method of claim 7, wherein said enzyme comprising deacetylase activity is selected from the group consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, and AcuC.
- 20 12. A method of evaluating the binding properties of the potential deacetylase inhibitor compound comprising the steps of:
 - a. co-crystallizing said compound with HDLP;
 - b. determining the three-dimensional structure of said HDLP-potential inhibitor complex co-crystal by molecular replacement using the three-dimensional structure of HDLP as defined by atomic coordinates according to Figure 16; and
 - 25 c. analyzing said three-dimensional structure of said HDLP bound to said potential inhibitor compound to evaluate the binding characteristics of said
 - 30 potential inhibitor compound.
13. A method for solving the structure of an HDAC family

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member crystal comprising the steps of:

- a. collecting X-ray diffraction data of said crystal wherein said data diffracts to a high resolution limit of greater than 4 Å;
 - 5 b. using the atomic coordinates of HDLP according to Figure 16 to perform molecular replacement or refinement and difference fourier with said X-ray diffraction data of said HDAC family member crystal to determine the structure of said HDAC family member; and
 - 10 c. refining said structure of said HDAC family member.
14. The method of claim 13, wherein said HDAC family member is HDAC1.
 - 15
 15. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant is encoded by the nucleic acid sequence of SEQ ID NO:4.
 - 20
 16. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant has the amino acid sequence of SEQ ID NO:3.
 17. A nucleotide sequence according to SEQ ID NO:4
 - 25
 18. An expression vector comprising the nucleotide sequence of claim 17.
 19. A method of using the crystal of claim 1 for screening
 - 30 for a novel drug comprising:
 - a. selecting a potential ligand by performing

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rational drug design with the three-dimensional structure determined for the crystal;

5. b. contacting the potential ligand with the ligand binding domain of the crystal; and

10 c. detecting the binding potential of the potential ligand for the ligand binding domain, wherein the novel drug is selected based on its having a greater affinity for the ligand binding domain than that of a known drug.

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Figure 1

TABLE 1. Statistics from the crystallographic analysis

| Data set | Native | thimerosal | Pb | AuCN | Zn | TSA | | |
|----------------------------|----------------------|-------------|-------------|--------------|------------|---|------------|----------------------------|
| Space Group | C2 | C2 | C2 | C2 | C2 | P2 ₁ 2 ₁ 2 ₁ | | |
| Resolution (Å) | 1.8 | 2.3 | 3.5 | 2.8 | 2.0 | 2.1 | | |
| Observations | 134,952 | 79,023 | 11,454 | 27,722 | 125,769 | 180,427 | | |
| Unique reflections | 32,143 | 15,958 | 4,040 | 8,753 | 23,643 | 50,796 | | |
| Data coverage (%) | 92.3 | 95.7 | 86.4 | 94.3 | 90.6 | 93.8 | | |
| R _{sym} (%) | 2.9 | 8.4 | 9.6 | 8.9 | 7.2 | 7.1 | | |
| MIR analysis (20.0-2.5 Å): | | | | | | | | |
| phasing power | - | 1.47 | 1.24 | 1.10 | - | - | | |
| R _{collis} | - | 0.72 | 0.78 | 0.85 | - | - | | |
| R _{collis} (ano) | - | 0.92 | | | - | - | | |
| Refinement statistics: | | | | | | RMSD | | |
| Data Set | Reflections | Total atoms | Water atoms | R-factor (%) | R-free (%) | bonds (Å) | angles (°) | B-factor (Å ²) |
| HDLP | (F > 1σ) 31,550 | 3214 | 228 | 19.8 | 24.0 | 0.010 | 1.63 | 3.55 |
| HDLP-Zn | 23,582 | 3424 | 434 | 22.0 | 25.8 | 0.009 | 1.48 | 1.04 |
| HDLP-Zn-TSA | 44,122 | 6475 | 456 | 22.4 | 25.8 | 0.008 | 1.78 | 3.83 |

$R_{\text{sym}} = \sum_h \sum_l |I_{h,l} - \langle I_h \rangle| / \sum_h \sum_l I_{h,l}$ for the intensity (I) of h observations of reflection h . Phasing power = $\langle F_{\text{calc}} \rangle / E$, where $\langle F_{\text{calc}} \rangle$ is the root-mean-square heavy atom structure factor and E is the residual lack of closure error. R_{collis} is the mean residual lack of closure error divided by the dispersive difference. R -factor = $\sum |F_{\text{obs}} - F_{\text{calc}}| / \sum |F_{\text{obs}}|$, where F_{obs} and F_{calc} are the observed and calculated structure factors, respectively. Figure of merit = $|F(hkl)_{\text{best}}| / |F(hkl)|$. R -free = R -factor calculated using 5% of the reflection data chosen randomly and omitted from the start of refinement. RMSD: root mean square deviations from ideal geometry and root mean square variation in the B-factor of bonded atoms.

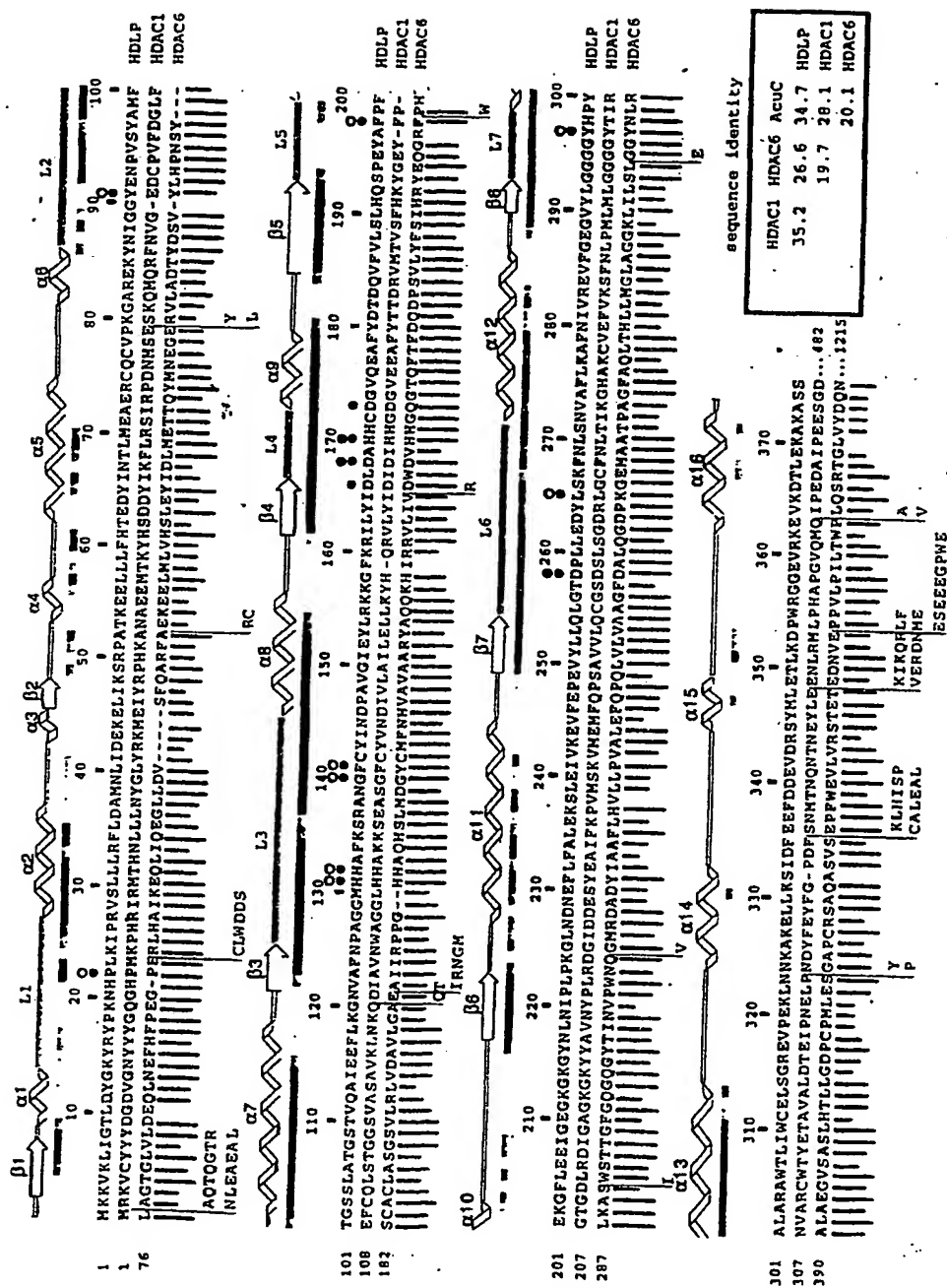


Figure 2

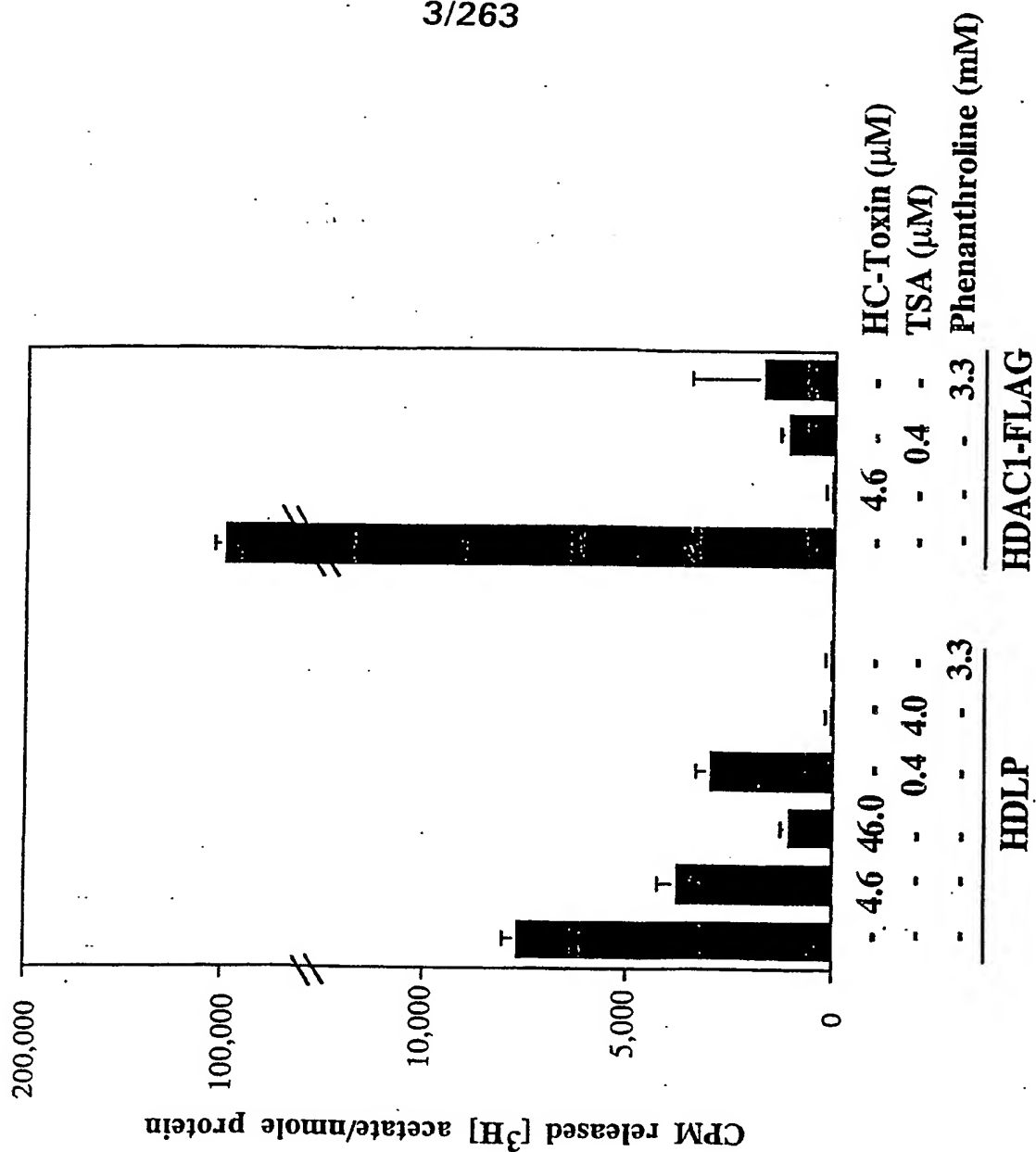
HDAC conservation solvent accessibility helix \rightarrow beta strand \rightarrow random coil
 high ||| exposed buried o in contact with TSA
 • zinc ligands
 • pocket residues
 - form the pocket

Figure 2

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Figure 3



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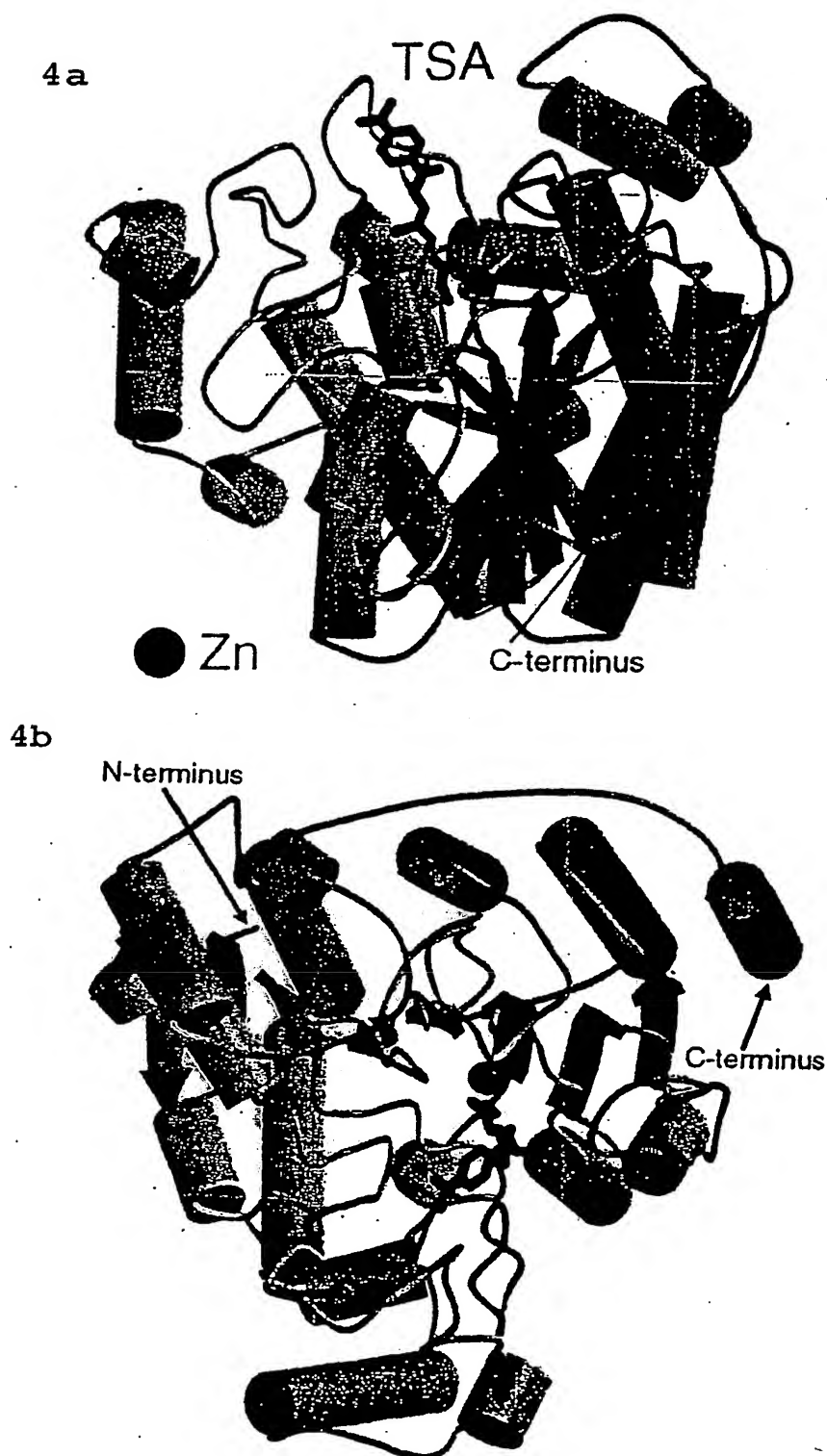
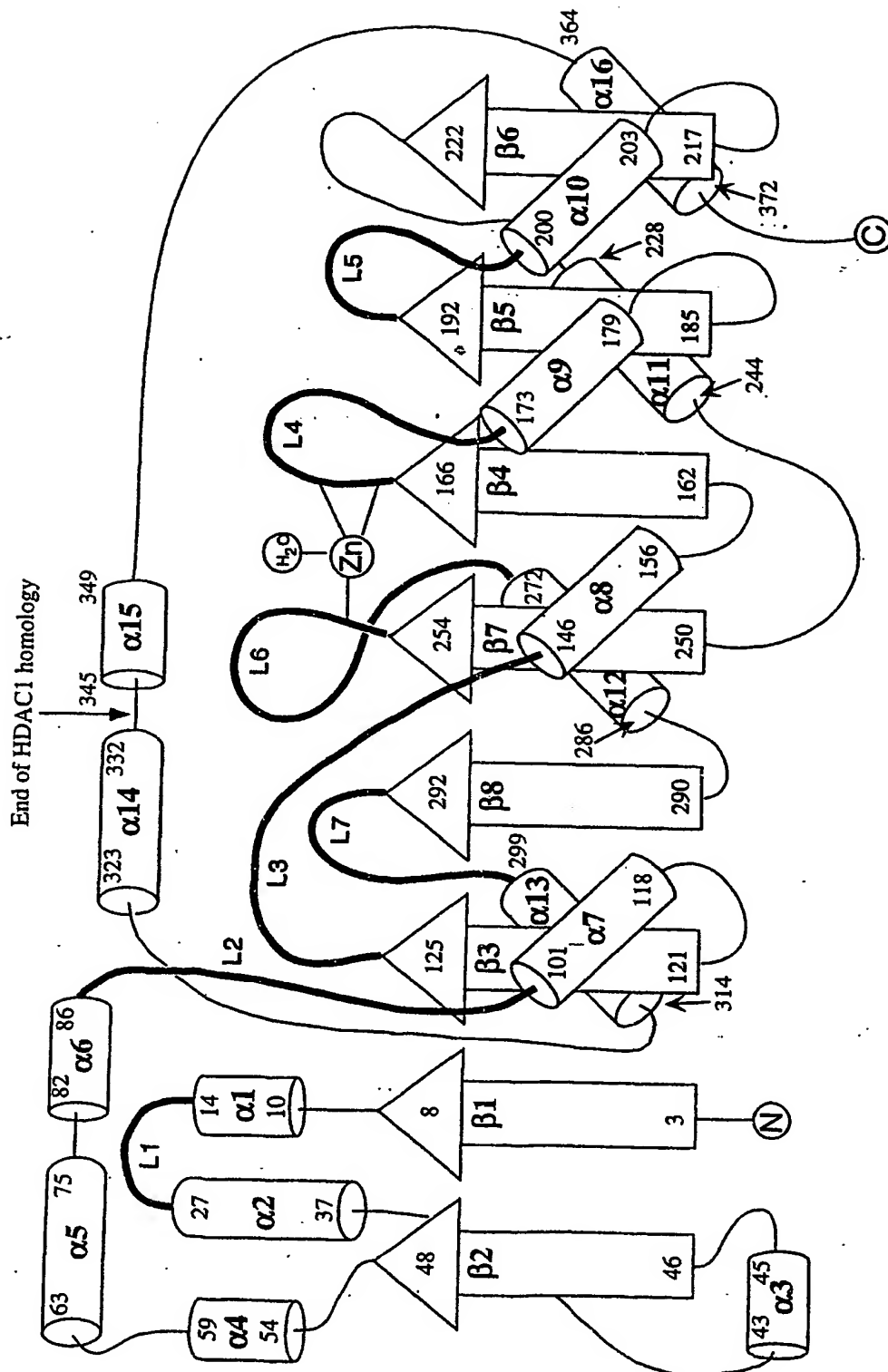


Figure 4

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Figure 4C



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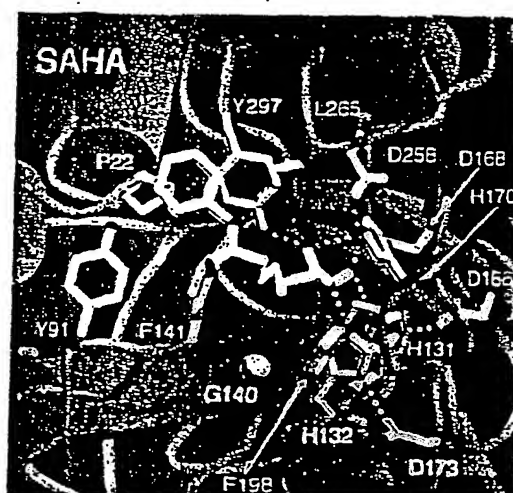
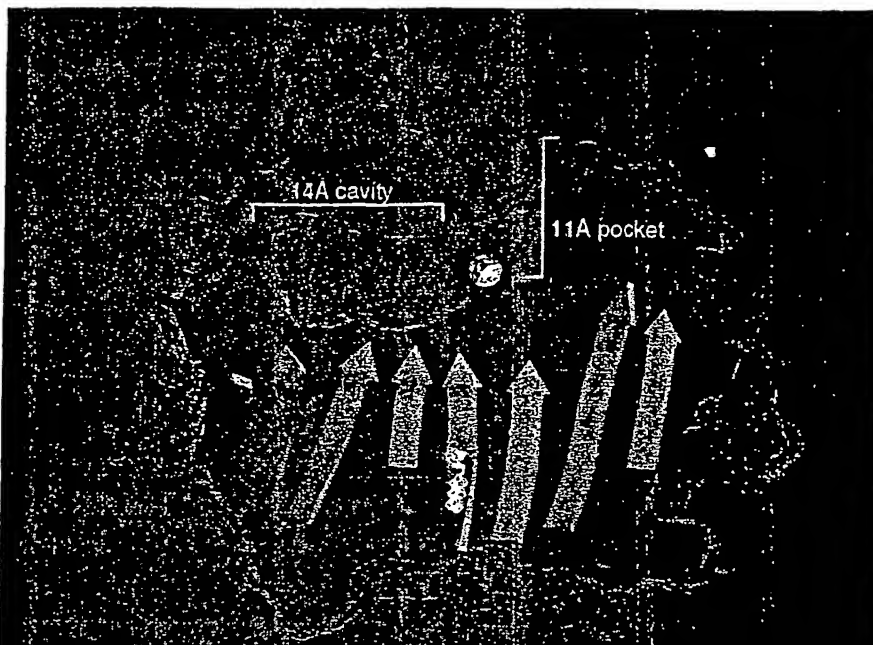


Figure 4D

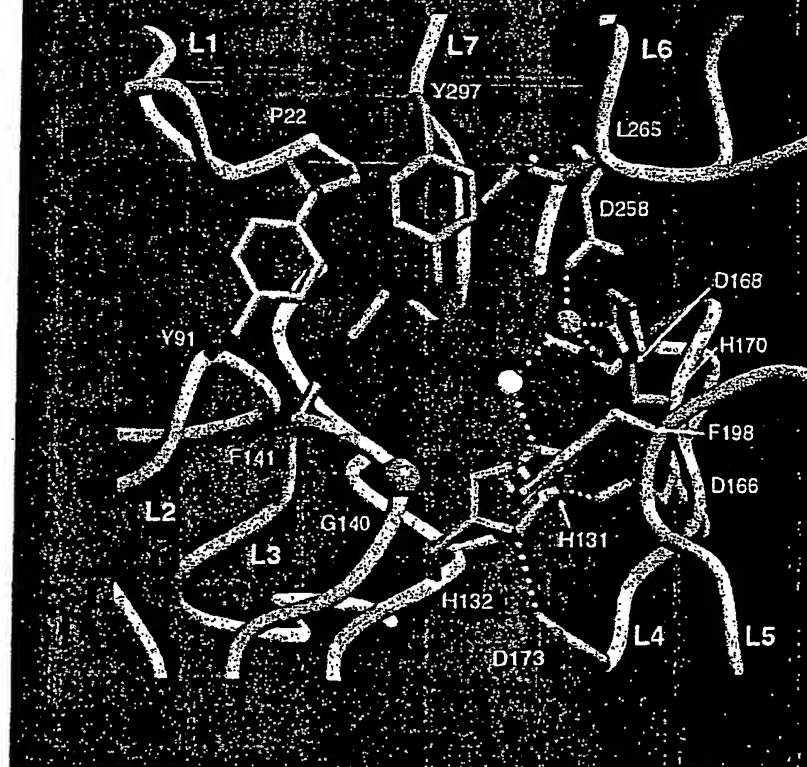
Figure 5

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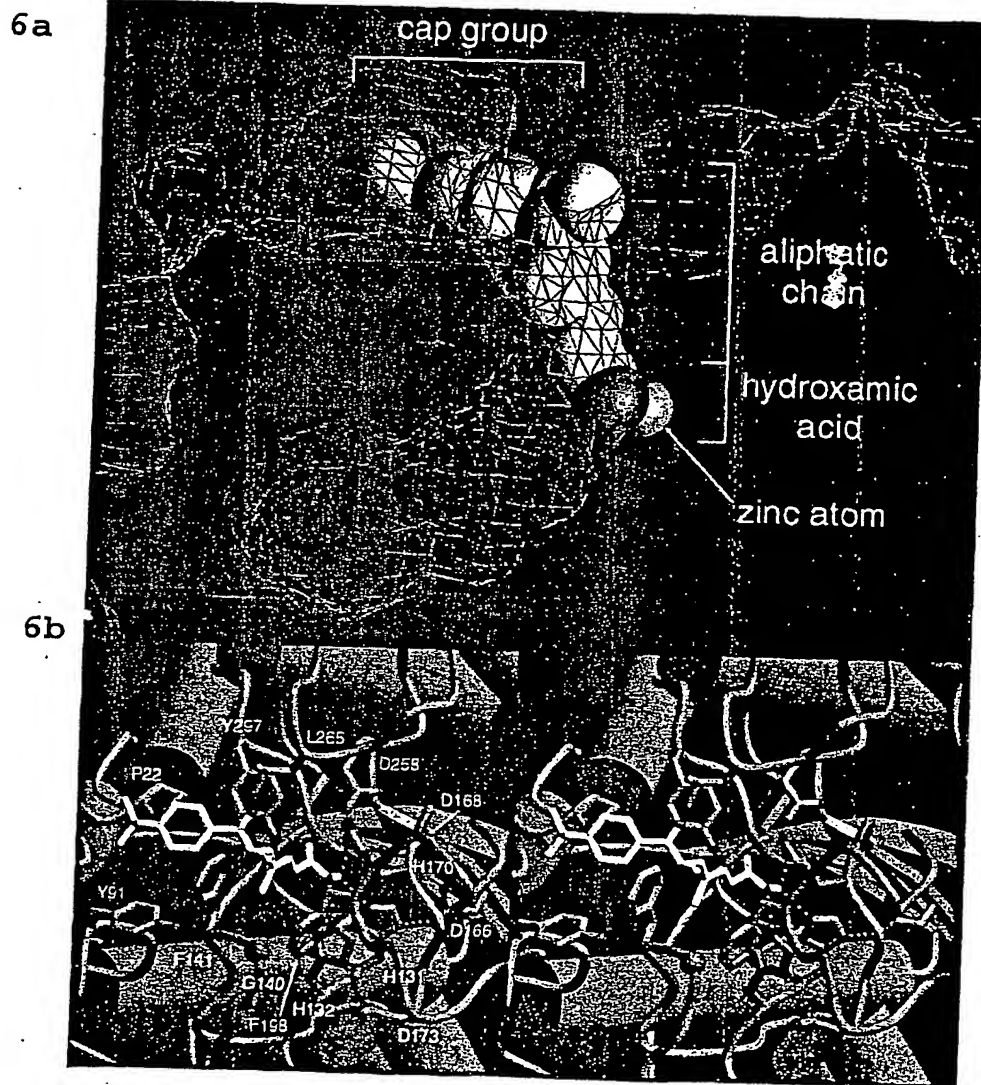
5b



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Figure 6



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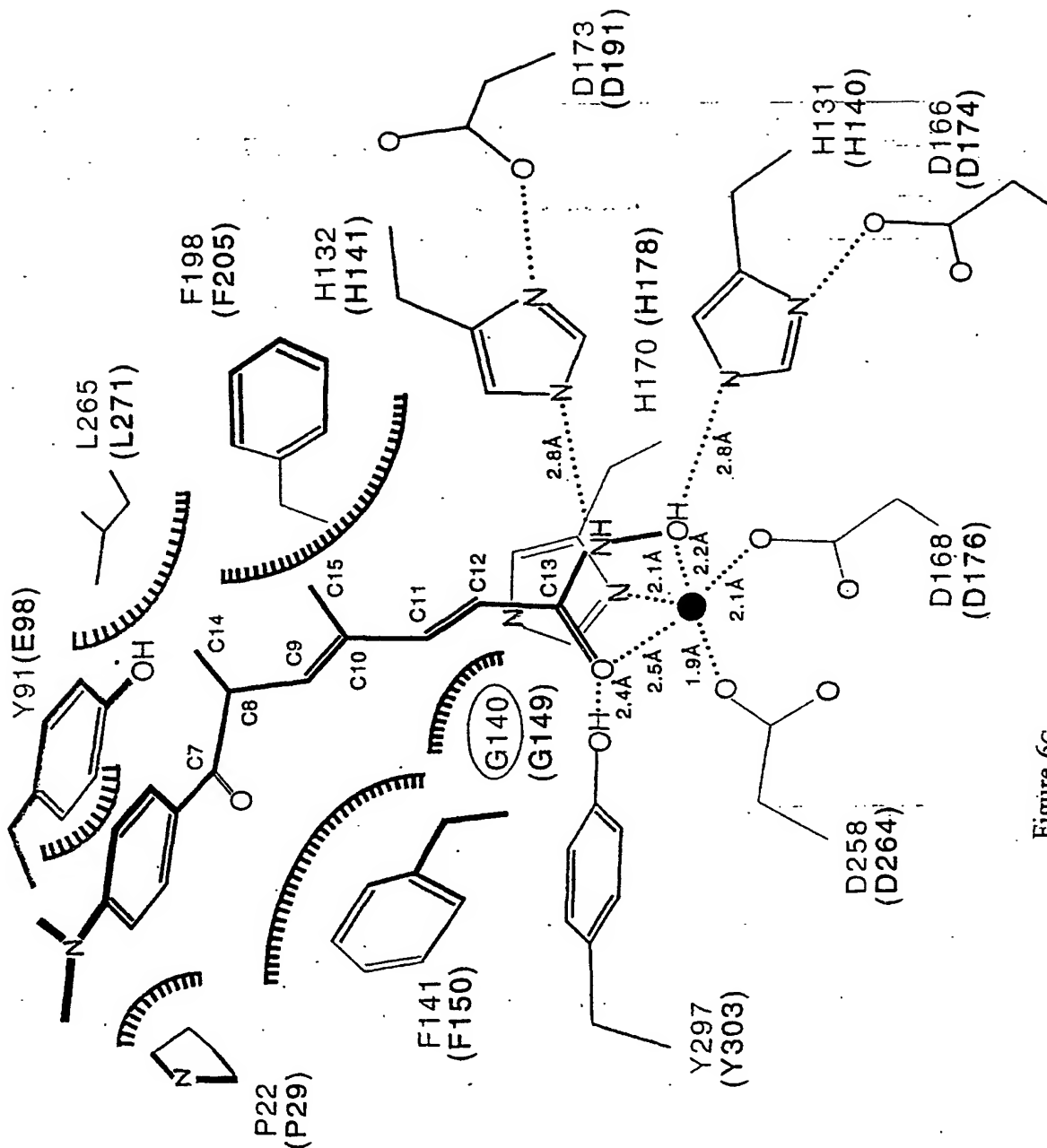
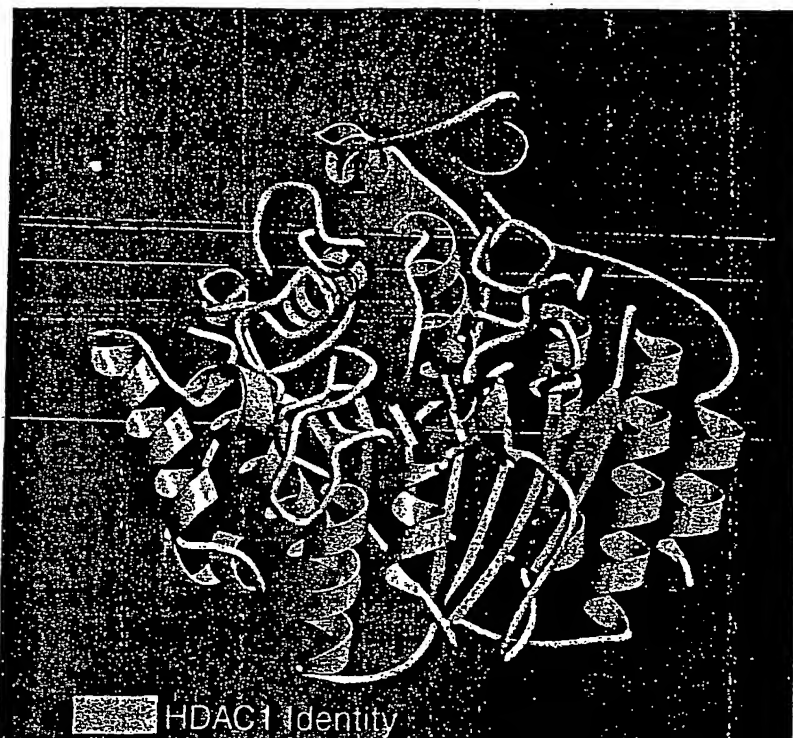


Figure 6C

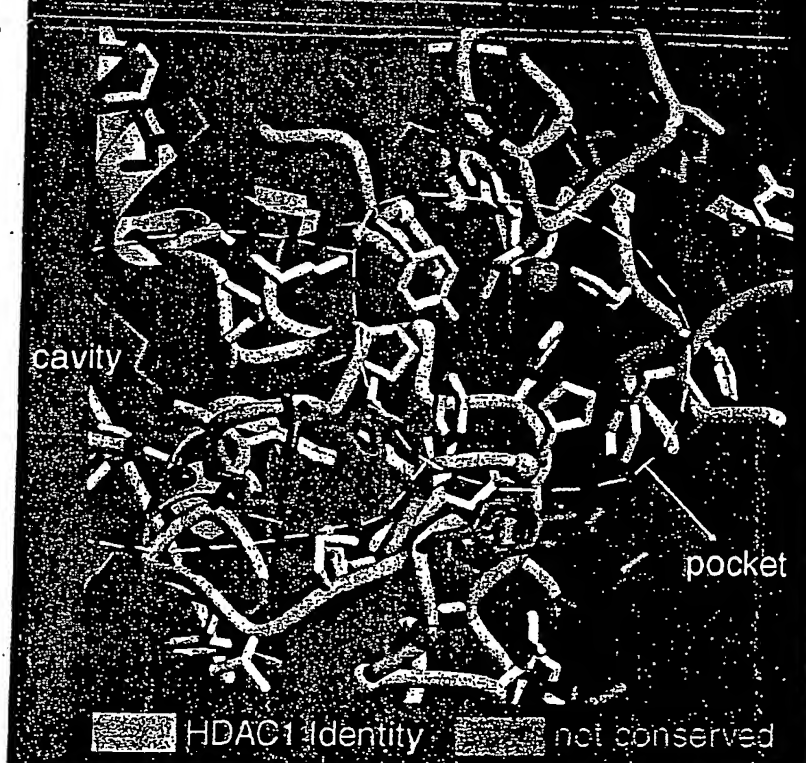
Figure 7

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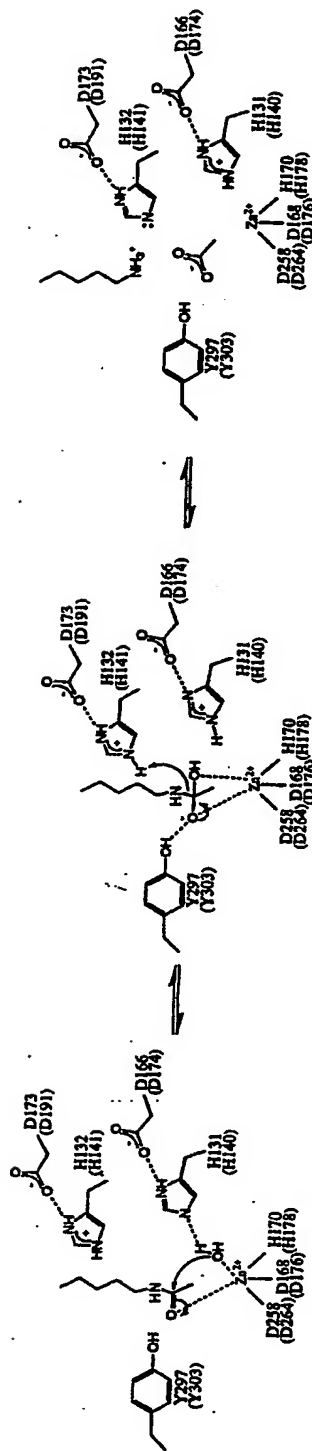


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Figure 8



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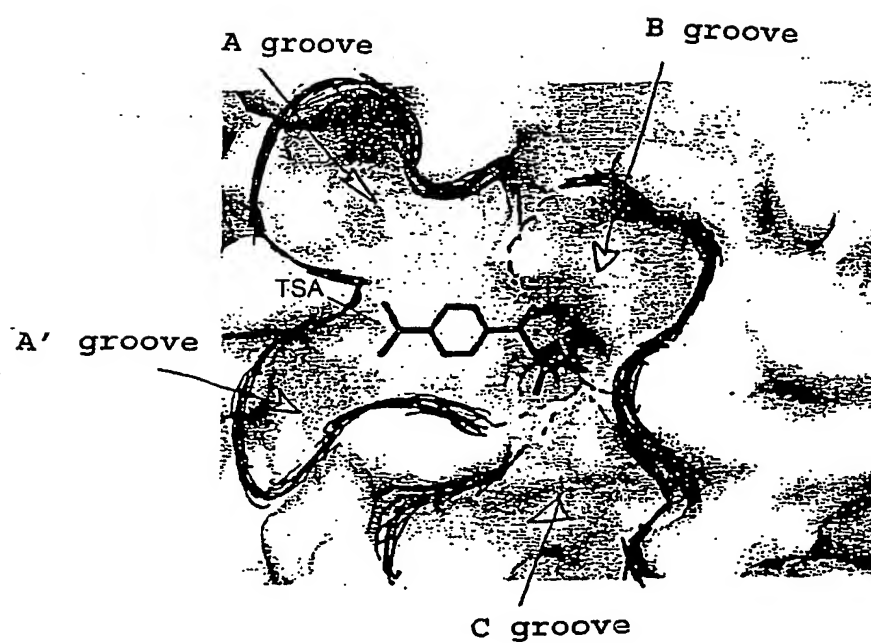


Figure 9

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Figure 10

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10 20 30 40
ATGAAGAAGGTTAACTTATCGGAACITTTAGACTACGGAA 40
AGTACAGATATCCCAAAAACCATCCTCTTAAAATACCAAG 80
AGTTTCCCTACTCCTTAGGTTTATTAGATGCCATGAACCTT 120
ATAGATGAGAAGGAATTAATCAAGAGCAGACCCGCAACTA 160
AAGAAGAACTCCTTTTATTCCACACGGAAGACTACATAAA 200

210 220 230 240
CACTTTAATGGAAGCGGAAAGGTGTCAGTGCGTTCCGAAG 240
GGAGCTAGGGAAAAGTACAACATAGGCGGATACGAAAACC 280
CCGTATCTTACGCGATGTTTACAGGCTCTTCTCTCGCAAC 320
GGGTTCAACAGTGCAGGCGATAGAGGAATTTTAAAGGGA 360
AATGTAGCTTTCAATCCCGCGGGAGGTATGCACCACGCTT 400

410 420 430 440
TTAAAGCAGGGCAAACGGCTTTTGCTACATAAACGACCC 440
CGCTGTGGGAATTGAGTACTTGAGAAAAAAGGCTTTAAG 480
AGAATACTCTACATAGACCTTGATGCCACCACCTGCGACG 520
GTGTTCAAGGAAGCCTTTTACGATACAGACCAGGTGTTTCT 560
CCTGTCCCTTCACCAGTCGCCCCGAGTACGCCCTTTCCCTTT 600

610 620 630 640
GAGAAGGGCTTCCTGGAGGAGATAGGAGAAGGAAAAGGAA 640
AGGGCTACAACCTGAACATTCCCCTGCCAAAGGGCTTGAA 680
CGACAACGAGTTCCCTCTTTGCCCTAGAAAAATCTCTGGAA 720
ATAGTCAAAGAAGTATTTGAGCCCGAGGTTTACCTTCTTC 760
AACTCGGAAGTGAACCACTCCTTGAAGATTACCTTTCCAA 800

810 820 830 840
GTTCAACCTCTCAAACGTTGCTTTTAAAAGCTTTCAAC 840
ATCGTTCTGTGAGGTTTTCGGGGAGGGAGTATACCTCGGAG 880
GAGGCGGATACCATCCTTACGCCCCGCAAGGGCATGGAC 920
CCTAAATCTGGTTCGAGCTTTTCGGGAAGGGAAGTGCCGGAA 960
AAGCTAAACAATAAAGCAAAAGAGCTTTTAAAGAGTATAG 1000

1010 1020 1030 1040
ACTTTGAAGAGTTTGACGACGAGGTGGACCGCTCGTACAT 1040
GCTCGAAACCCCTAAAGGACCCCTGGAGAGGAGGAGAGGTA 1080
AGGAAAGAAGTAAAGGATACGCTTGAAAAGGCGAAAGCCT 1120
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Figure 11

10 20 30 40
MKKVKLIGTLDYGKYRYPKNHPLKIPRVSLLLRFLDAMNL 40
IDKELIKSRPATKEELLLFHTEDYINTLMEAERCQCVPK 80
GAREKYNIGGYENPVSYAMFTGSSLATGSTVQAIEEFLKG 120
NVAENPAGGMHAFKSRANGFCYINDPAVGIEYLRKKGFK 160
RILYIDLDAHHCDCGVQEAIFYDFDQVFVLSLHQSPEYAFPF 200
210 220 230 240
EKGFLLEIGEGKGKGYNLNIPLPKGLNDNEFLFALEKSLE 240
IVKEVFEPEVYLLQLGTDPLLEDYLSKFNL SNVAFLKAFN 280
IVREVFEGGVYLGGGGYHPYALARAWTLIWCELSGREVPE 320
KLNNKAKELLKSIDFEEFDDEVDRSYMLETLKDPWRGGEV 360
RKEVKDTLEKAKASS 375

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Figure 12

10 20 30 40
ATGAAGAAGGTTAACTTATCGGAACCTTAGACTACGGAA 40
AGTACAGATATCCCAAAAACCATCCTCTTAAAATACCAAG 80
AGTTTCCCTACTCCTTAGGTTTTTAGATGCCATGAACCTT 120
ATAGATGAGAAGGAATTAATCAAGAGCAGACCCGCAACTA 160
AAGAAGAACTCCCTTTTATTCACACGGAAGACTACATAAA 200
210 220 230 240
CACTTTAATGGAAGCGGAAAGGTGTCAGTGGTTCCTGAAG 240
GGAGCTAGGGAAAAGTACAACATAGGCGGATACGAAAACC 280
CCGTATCTTACGCGATGTTTACAGGCTCTTCTCTCGCAAC 320
GGGTTCAACAGTGCAGGCGATAGAGGAATTTTAAAGGGA 360
AATGTAGCTTTCAATCCCGCGGAGGTATGCACCACGCTT 400
410 420 430 440
TTAAAAGCAGGGCAAACGGCTTTTGCTACATAAAACGACCC 440
CGCTGTGGGAATTGAGTACTTGAGAAAAAAGGCTTTAAG 480
AGAATACTCTACATAGACCTTGATGCCCCACCACTGCGACG 520
GTGTTTCAAGGAAGCCTTTTACGATACAGACCAGGTGTTCTG 560
CCTGTCCCTTCACCAGTCGCCCCGAGTACGCTTTCCCTTT 600
610 620 630 640
GAGAAGGGCTTCCTGGAGGAGATAGGAGAAGGAAAAGGAA 640
AGGGCTACAACCTGAACATTCCCCTGCCAAAGGGCTTGAA 680
CGACAACGAGTTCTCTTTTGCCCTAGAAAAATCTCTGGAA 720
ATAGTCAAAGAAGTATTTGAGCCCGAGGTTTACCTTCTTC 760
AACTCGGAACGACCCACTCCTTGAAGATTACCTTTCCAA 800
810 820 830 840
GTTCAACCTCTCAAACGTTGCCTTTTTTAAAAGCTTTCAAC 840
ATCGTTTCGTGAGGTTTTTCGGGGAGGGAGTATACCTCGGAG 880
GAGGCGGATTCCATCCTTACGCCCTCGCAAGGGCATGGAC 920
CCTAATCTGGTGGAGCTTTTCGGGAAGGGAAGTGCCGGAA 960
AAGCTAAACAATAAAGCAAAAGAGCTTTTAAAGAGTATAG 1000
1010 1020 1030 1040
ACTTTGAAGAGTTTGACGACGAGGTGGACCGCTCGTACAT 1040
GCTCGAAACCTTAAAGGACCCCTGGAGAGGAGGAGAGGTA 1080
AGGAAAGAAGTAAAGGATACGCTTTGAAAAGGCGAAAGCCT 1120
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Figure 13

10 20 30 40

MKKVKLIGTLDYGKYRYPKNHPLKIPRVSLLLRFLDAMNL 40
IDKELIKSRPATKEELLLFHTEDYINTLMEAEQCQCVPK 80
GAREKYNIGGYENFVSAMFTGSSLATGSTVQATEEFLKG 120
NVAFNPAGGMHHAFKSRANGFCYINDPAVGIEYLRKKGFK 160
RTLYIDLDAHHCDCGVQEAIFYDIDQVFVLSLHQSPYAFPF 200

210 220 230 240

EKGFL EEIGEGKGKGYNLNIPLPKGLNDNEFLFALEKSLE 240
IVKEVFEPEVYLLQLGTDPLLEDYLSKFNL SNVAFLKAFN 280
IVREVFGEVYLG GGGFHPYALARAWTLIWCELSGREVPE 320
KLNNKAKELLKSIDFEEFDDEVDRSYMLETLKDPWRGGEV 360
RKEVKDILEKAKASS 375

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Figure 14

10 20 30 40
ATGAAGAAGGTTAAACTTATCGGAACTTTAGACTACGGAA 40
AGTACAGATATCCCAAAAACCATCCTCTTAAAAATACCAAG 80
AGTTTCCCTACTCCTTAGGTTTTTAGATGCCATGAACCTT 120
ATAGATGAGAAGGAATTAATCAAGAGCAGACCCGCAACTA 160
AAGAAGAACTCCTTTTATTCCACACGGAAGACTACATAAA 200
210 220 230 240
CACTTTAATGGAAGCGGAAAGGAGTCAGAGCGTTCCGAAG 240
GGAGCTAGGGGAAAAGTACAACATAGGCGGATACGAAAACC 280
CCGTATCTTACGCGATGTTTACAGGCTCTTCTCTCGCAAC 320
GGGTTCAACAGTGCAGGCGATAGAGGAATTTTAAAGGGA 360
AATGTAGCTTTCAATCCCGCGGGAGGTATGCACCACGCTT 400
410 420 430 440
TTAAAAGCAGGGCAAACGGCTTTTGCTACATAAACGACCC 440
CGCTGTGGGAATTGAGTACTTGAGAAAAAAGGCTTTAAG 480
AGAATACTCTACATAGACCTTGATGCCCACTGCGACG 520
GTGTTCAAGGAAGCCTTTTACGATACAGACCAGGTGTTGCT 560
CCTGTCCCTTTCACCAGTCGCCCCGAGTACGCCTTTCCCTTT 600
610 620 630 640
GAGAAGGGCTTCCTGGAGGAGATAGGAGAAGGAAAAGGAA 640
AGGGCTACAACCTGAACATTTCCCTTGCCAAAGGGCTTGAA 680
CGACAACGAGTTCTCTTTTGCCCTAGAAAAA/CTCTGGAA 720
ATAGTCAAAGAAGTATTTGAGCCCGAGGTTTACCTTCTTC 760
AACTCGGAACCTGACCCACTCCTTGAAGATTACCTTTCCAA 800
810 820 830 840
GTTCAACCTCTCAAACGTTGCTTTTAAAAAGCTTTCAAC 840
ATCGTTCTGTGAGGTTTTCGGGGAGGGAGTATACCTCGGAG 880
GAGGCGGATACCATCCTTACGCCCTCGCAAGGGCATGGAC 920
CCTAATCTGGTGCAGCTTTTCGGGAAGGGAAGTGCCGGAA 960
AAGCTAAACAATAAAGCAAAAGAGCTTTTAAAGAGTATAG 1000
1010 1020 1030 1040
ACTTTGAAGAGTTTGACGACGAGGTGGACCGCTCGTACAT 1040
GCTCGAAACCCCTAAAGGACCCCTGGAGAGGAGGAGAGGTA 1080
AGGAAAGAAGTAAAGGATACGCTTGAAAAGGCGAAAGCCT 1120
CATCTTA 1127

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Figure 15

10 20 30 40
MKKVKLIGTLDYGKYRYPKNHPLKIPRVSLLLRFLDAMNL 40
IDKELIKSRPATKEELLLFHTEDYINTIMEAERSQSVPK 80
GAREKYNIGGYENPVSYAMFTGSSLATGSTVQAIEEFLKG 120
NVAFNPAAGGMHHAFKSRANGFCYINDPAVGIEYLRKKGFK 160
RILYIDLLDAHCDGVQEAIFYDTDQVFVLSLHQSPYAFPF 200
210 220 230 240
EKGFLFEEIGEGKGKGYNLNIPKGLNDNEFLFALEKSLE 240
IVKEVFEPEVYLLQLGTDPLLEDYLSKFNLNVAFLKAFN 280
IVREVFGEVYLGGGGYHPYALARAWTLIWCELSGREVPE 320
KLNNKAKELLKSIDFEEFDDEVDRSYMLETCLKDPWRGGEV 360
RKEVKDTLEKAKASS 375

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Figure 16-1

| | | | | Residue # | X | Y | Z | OCC. | B | Segment ID |
|------|----|-----|-----|-----------|--------|--------|--------|------|-------|------------|
| ATOM | 1 | CB | ALA | 2 | 45.336 | 36.880 | 73.042 | 1.00 | 59.90 | AAAA |
| ATOM | 2 | C | ALA | 2 | 46.410 | 38.631 | 73.628 | 1.00 | 52.57 | AAAA |
| ATOM | 3 | O | ALA | 2 | 45.780 | 39.595 | 74.052 | 1.00 | 62.46 | AAAA |
| ATOM | 4 | N | ALA | 2 | 47.540 | 37.826 | 75.673 | 1.00 | 58.52 | AAAA |
| ATOM | 5 | CA | ALA | 2 | 46.668 | 37.432 | 74.527 | 1.00 | 57.32 | AAAA |
| ATOM | 6 | N | LYS | 3 | 46.890 | 38.570 | 72.389 | 1.00 | 39.61 | AAAA |
| ATOM | 7 | CA | LYS | 3 | 46.687 | 39.669 | 71.440 | 1.00 | 29.58 | AAAA |
| ATOM | 8 | CB | LYS | 3 | 47.855 | 39.763 | 73.459 | 1.00 | 36.03 | AAAA |
| ATOM | 9 | CG | LYS | 3 | 49.227 | 40.007 | 72.102 | 1.00 | 55.16 | AAAA |
| ATOM | 10 | CD | LYS | 3 | 50.315 | 40.000 | 73.039 | 1.00 | 66.29 | AAAA |
| ATOM | 11 | CE | LYS | 3 | 51.700 | 40.163 | 73.655 | 1.00 | 73.41 | AAAA |
| ATOM | 12 | NZ | LYS | 3 | 52.791 | 40.047 | 69.642 | 1.00 | 69.64 | AAAA |
| ATOM | 13 | C | LYS | 3 | 45.407 | 39.422 | 70.642 | 1.00 | 23.29 | AAAA |
| ATOM | 14 | O | LYS | 3 | 44.984 | 38.282 | 70.487 | 1.00 | 27.41 | AAAA |
| ATOM | 15 | N | VAL | 4 | 44.814 | 40.498 | 70.138 | 1.00 | 25.18 | AAAA |
| ATOM | 16 | CA | VAL | 4 | 43.585 | 40.418 | 69.349 | 1.00 | 22.20 | AAAA |
| ATOM | 17 | CB | VAL | 4 | 42.501 | 41.365 | 69.887 | 1.00 | 21.46 | AAAA |
| ATOM | 18 | CG1 | VAL | 4 | 41.214 | 41.202 | 69.066 | 1.00 | 26.55 | AAAA |
| ATOM | 19 | CG2 | VAL | 4 | 42.244 | 41.080 | 71.348 | 1.00 | 34.98 | AAAA |
| ATOM | 20 | C | VAL | 4 | 43.983 | 40.851 | 67.961 | 1.00 | 25.33 | AAAA |
| ATOM | 21 | O | VAL | 4 | 44.557 | 41.927 | 67.778 | 1.00 | 21.19 | AAAA |
| ATOM | 22 | N | LYS | 5 | 43.654 | 40.023 | 66.978 | 1.00 | 21.32 | AAAA |
| ATOM | 23 | CA | LYS | 5 | 44.052 | 40.291 | 65.607 | 1.00 | 20.10 | AAAA |
| ATOM | 24 | CB | LYS | 5 | 45.047 | 39.214 | 65.177 | 1.00 | 23.35 | AAAA |
| ATOM | 25 | CG | LYS | 5 | 46.301 | 39.092 | 66.049 | 1.00 | 23.75 | AAAA |
| ATOM | 26 | CD | LYS | 5 | 47.183 | 40.334 | 65.919 | 1.00 | 23.70 | AAAA |
| ATOM | 27 | CE | LYS | 5 | 48.510 | 40.151 | 66.669 | 1.00 | 24.34 | AAAA |
| ATOM | 28 | NZ | LYS | 5 | 49.351 | 41.387 | 66.585 | 1.00 | 22.04 | AAAA |
| ATOM | 29 | C | LYS | 5 | 42.914 | 40.294 | 64.596 | 1.00 | 20.27 | AAAA |
| ATOM | 30 | O | LYS | 5 | 41.949 | 39.535 | 64.728 | 1.00 | 18.48 | AAAA |
| ATOM | 31 | N | LEU | 6 | 43.071 | 41.111 | 63.564 | 1.00 | 19.28 | AAAA |
| ATOM | 32 | CA | LEU | 6 | 42.097 | 41.156 | 62.483 | 1.00 | 20.68 | AAAA |
| ATOM | 33 | CB | LEU | 6 | 41.571 | 42.574 | 62.291 | 1.00 | 23.51 | AAAA |
| ATOM | 34 | CG | LEU | 6 | 40.373 | 42.712 | 61.342 | 1.00 | 30.59 | AAAA |
| ATOM | 35 | CD1 | LEU | 6 | 40.079 | 44.192 | 61.153 | 1.00 | 29.90 | AAAA |
| ATOM | 36 | CD2 | LEU | 6 | 40.657 | 42.085 | 59.995 | 1.00 | 36.98 | AAAA |
| ATOM | 37 | C | LEU | 6 | 42.954 | 40.701 | 61.237 | 1.00 | 18.17 | AAAA |
| ATOM | 38 | O | LEU | 6 | 43.911 | 41.249 | 60.919 | 1.00 | 22.31 | AAAA |
| ATOM | 39 | N | ILE | 7 | 42.359 | 39.689 | 60.538 | 1.00 | 19.15 | AAAA |
| ATOM | 40 | CA | ILE | 7 | 43.045 | 39.199 | 59.338 | 1.00 | 18.38 | AAAA |
| ATOM | 41 | CE | ILE | 7 | 42.922 | 37.674 | 59.191 | 1.00 | 19.05 | AAAA |
| ATOM | 42 | CG2 | ILE | 7 | 43.930 | 37.162 | 59.144 | 1.00 | 16.45 | AAAA |
| ATOM | 43 | CG1 | ILE | 7 | 43.253 | 37.007 | 60.521 | 1.00 | 22.81 | AAAA |
| ATOM | 44 | CD1 | ILE | 7 | 43.286 | 35.543 | 60.450 | 1.00 | 34.99 | AAAA |
| ATOM | 45 | C | ILE | 7 | 42.396 | 39.850 | 58.125 | 1.00 | 17.95 | AAAA |
| ATOM | 46 | O | ILE | 7 | 41.188 | 39.729 | 57.928 | 1.00 | 19.07 | AAAA |
| ATOM | 47 | N | GLY | 8 | 43.193 | 40.562 | 57.330 | 1.00 | 17.70 | AAAA |
| ATOM | 48 | CA | GLY | 8 | 42.623 | 41.193 | 56.148 | 1.00 | 18.11 | AAAA |
| ATOM | 49 | C | GLY | 8 | 43.640 | 41.857 | 55.243 | 1.00 | 20.91 | AAAA |
| ATOM | 50 | O | GLY | 8 | 44.849 | 41.840 | 55.504 | 1.00 | 22.27 | AAAA |
| ATOM | 51 | N | THR | 9 | 43.134 | 42.428 | 54.155 | 1.00 | 23.99 | AAAA |
| ATOM | 52 | CA | THR | 9 | 43.950 | 43.141 | 53.183 | 1.00 | 25.95 | AAAA |
| ATOM | 53 | CB | THR | 9 | 44.739 | 42.195 | 52.263 | 1.00 | 25.80 | AAAA |
| ATOM | 54 | CG1 | THR | 9 | 45.321 | 42.962 | 51.199 | 1.00 | 26.56 | AAAA |
| ATOM | 55 | CG2 | THR | 9 | 43.823 | 41.144 | 51.657 | 1.00 | 25.24 | AAAA |
| ATOM | 56 | C | THR | 9 | 43.025 | 43.957 | 52.294 | 1.00 | 29.04 | AAAA |
| ATOM | 57 | O | THR | 9 | 41.872 | 43.582 | 52.082 | 1.00 | 23.05 | AAAA |
| ATOM | 58 | N | LEU | 10 | 43.517 | 45.079 | 51.781 | 1.00 | 29.19 | AAAA |
| ATOM | 59 | CA | LEU | 10 | 42.690 | 45.896 | 50.895 | 1.00 | 32.55 | AAAA |
| ATOM | 60 | CB | LEU | 10 | 43.256 | 47.319 | 50.761 | 1.00 | 28.09 | AAAA |
| ATOM | 61 | CG | LEU | 10 | 43.142 | 48.256 | 51.958 | 1.00 | 33.00 | AAAA |
| ATOM | 62 | CD1 | LEU | 10 | 41.680 | 48.403 | 52.347 | 1.00 | 26.65 | AAAA |
| ATOM | 63 | CD2 | LEU | 10 | 43.938 | 47.744 | 53.126 | 1.00 | 41.33 | AAAA |
| ATOM | 64 | C | LEU | 10 | 42.566 | 45.261 | 49.512 | 1.00 | 32.68 | AAAA |
| ATOM | 65 | O | LEU | 10 | 41.736 | 45.684 | 48.702 | 1.00 | 26.97 | AAAA |
| ATOM | 66 | N | ASP | 11 | 43.377 | 44.234 | 49.256 | 1.00 | 25.75 | AAAA |

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Figure 16-2

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 67 | CA | ASP | 11 | 43.367 | 43.541 | 47.970 | 1.00 | 35.74 | AAAA |
| ATOM | 68 | CB | ASP | 11 | 44.477 | 42.485 | 47.922 | 1.00 | 37.61 | AAAA |
| ATOM | 69 | CG | ASP | 11 | 45.858 | 43.093 | 48.079 | 1.00 | 46.75 | AAAA |
| ATOM | 70 | OD1 | ASP | 11 | 46.110 | 44.136 | 47.444 | 1.00 | 46.34 | AAAA |
| ATOM | 71 | OD2 | ASP | 11 | 46.690 | 42.528 | 48.821 | 1.00 | 58.94 | AAAA |
| ATOM | 72 | C | ASP | 11 | 42.034 | 42.898 | 47.607 | 1.00 | 34.26 | AAAA |
| ATOM | 73 | O | ASP | 11 | 41.748 | 42.696 | 46.420 | 1.00 | 31.12 | AAAA |
| ATOM | 74 | N | TYR | 12 | 41.220 | 42.558 | 48.609 | 1.00 | 26.19 | AAAA |
| ATOM | 75 | CA | TYR | 12 | 39.923 | 41.963 | 48.314 | 1.00 | 28.45 | AAAA |
| ATOM | 76 | CB | TYR | 12 | 39.119 | 41.720 | 49.601 | 1.00 | 29.35 | AAAA |
| ATOM | 77 | CG | TYR | 12 | 39.648 | 40.595 | 50.470 | 1.00 | 28.47 | AAAA |
| ATOM | 78 | CD1 | TYR | 12 | 40.137 | 40.846 | 51.755 | 1.00 | 32.17 | AAAA |
| ATOM | 79 | CE1 | TYR | 12 | 40.592 | 39.808 | 52.572 | 1.00 | 30.35 | AAAA |
| ATOM | 80 | CD2 | TYR | 12 | 39.629 | 39.276 | 50.017 | 1.00 | 22.97 | AAAA |
| ATOM | 81 | CE2 | TYR | 12 | 40.077 | 38.228 | 50.822 | 1.00 | 19.60 | AAAA |
| ATOM | 82 | CZ | TYR | 12 | 40.554 | 38.499 | 52.096 | 1.00 | 21.42 | AAAA |
| ATOM | 83 | OH | TYR | 12 | 40.964 | 37.456 | 52.907 | 1.00 | 23.49 | AAAA |
| ATOM | 84 | C | TYR | 12 | 39.144 | 42.907 | 47.390 | 1.00 | 26.67 | AAAA |
| ATOM | 85 | O | TYR | 12 | 38.307 | 42.466 | 46.593 | 1.00 | 30.51 | AAAA |
| ATOM | 86 | N | GLY | 13 | 39.441 | 44.201 | 47.492 | 1.00 | 30.22 | AAAA |
| ATOM | 87 | CA | GLY | 13 | 38.767 | 45.203 | 46.675 | 1.00 | 25.13 | AAAA |
| ATOM | 88 | C | GLY | 13 | 38.911 | 45.009 | 45.177 | 1.00 | 27.31 | AAAA |
| ATOM | 89 | O | GLY | 13 | 38.096 | 45.522 | 44.415 | 1.00 | 29.38 | AAAA |
| ATOM | 90 | N | LYS | 14 | 39.937 | 44.269 | 44.755 | 1.00 | 33.56 | AAAA |
| ATOM | 91 | CA | LYS | 14 | 40.176 | 44.005 | 43.337 | 1.00 | 39.81 | AAAA |
| ATOM | 92 | CB | LYS | 14 | 41.680 | 44.026 | 43.031 | 1.00 | 51.10 | AAAA |
| ATOM | 93 | CG | LYS | 14 | 42.292 | 45.424 | 42.907 | 1.00 | 64.99 | AAAA |
| ATOM | 94 | CD | LYS | 14 | 41.757 | 46.218 | 41.692 | 1.00 | 72.74 | AAAA |
| ATOM | 95 | CE | LYS | 14 | 42.183 | 45.639 | 40.336 | 1.00 | 67.25 | AAAA |
| ATOM | 96 | NZ | LYS | 14 | 41.637 | 44.280 | 40.045 | 1.00 | 70.06 | AAAA |
| ATOM | 97 | C | LYS | 14 | 39.589 | 42.688 | 42.834 | 1.00 | 39.98 | AAAA |
| ATOM | 98 | O | LYS | 14 | 39.746 | 42.350 | 41.658 | 1.00 | 46.99 | AAAA |
| ATOM | 99 | N | TYR | 15 | 38.927 | 41.944 | 43.717 | 1.00 | 32.64 | AAAA |
| ATOM | 100 | CA | TYR | 15 | 38.318 | 40.655 | 43.355 | 1.00 | 41.01 | AAAA |
| ATOM | 101 | CB | TYR | 15 | 38.996 | 39.512 | 44.126 | 1.00 | 26.48 | AAAA |
| ATOM | 102 | CG | TYR | 15 | 40.496 | 39.571 | 44.033 | 1.00 | 34.97 | AAAA |
| ATOM | 103 | CD1 | TYR | 15 | 41.289 | 39.401 | 45.167 | 1.00 | 43.28 | AAAA |
| ATOM | 104 | CE1 | TYR | 15 | 42.677 | 39.548 | 45.106 | 1.00 | 36.05 | AAAA |
| ATOM | 105 | CD2 | TYR | 15 | 41.127 | 39.879 | 42.827 | 1.00 | 40.78 | AAAA |
| ATOM | 106 | CE2 | TYR | 15 | 42.508 | 40.027 | 42.756 | 1.00 | 37.13 | AAAA |
| ATOM | 107 | CZ | TYR | 15 | 43.275 | 39.865 | 43.899 | 1.00 | 36.87 | AAAA |
| ATOM | 108 | OH | TYR | 15 | 44.644 | 40.044 | 43.844 | 1.00 | 35.40 | AAAA |
| ATOM | 109 | C | TYR | 15 | 36.838 | 40.705 | 43.714 | 1.00 | 38.62 | AAAA |
| ATOM | 110 | O | TYR | 15 | 36.344 | 39.868 | 44.468 | 1.00 | 37.82 | AAAA |
| ATOM | 111 | N | ARG | 16 | 36.141 | 41.703 | 43.177 | 1.00 | 44.85 | AAAA |
| ATOM | 112 | CA | ARG | 16 | 34.716 | 41.890 | 43.431 | 1.00 | 45.75 | AAAA |
| ATOM | 113 | CB | ARG | 16 | 34.320 | 43.348 | 43.187 | 1.00 | 54.17 | AAAA |
| ATOM | 114 | CG | ARG | 16 | 35.170 | 44.399 | 43.875 | 1.00 | 66.77 | AAAA |
| ATOM | 115 | CD | ARG | 16 | 34.920 | 44.506 | 45.369 | 1.00 | 72.39 | AAAA |
| ATOM | 116 | NE | ARG | 16 | 35.649 | 45.646 | 45.923 | 1.00 | 85.39 | AAAA |
| ATOM | 117 | CZ | ARG | 16 | 35.489 | 46.906 | 45.518 | 1.00 | 81.94 | AAAA |
| ATOM | 118 | NH1 | ARG | 16 | 34.624 | 47.197 | 44.554 | 1.00 | 80.19 | AAAA |
| ATOM | 119 | NH2 | ARG | 16 | 36.205 | 47.878 | 46.069 | 1.00 | 85.46 | AAAA |
| ATOM | 120 | C | ARG | 16 | 33.915 | 41.029 | 42.460 | 1.00 | 43.50 | AAAA |
| ATOM | 121 | O | ARG | 16 | 34.400 | 40.667 | 41.385 | 1.00 | 38.62 | AAAA |
| ATOM | 122 | N | TYR | 17 | 32.689 | 40.692 | 42.833 | 1.00 | 32.68 | AAAA |
| ATOM | 123 | CA | TYR | 17 | 31.850 | 39.923 | 41.930 | 1.00 | 37.55 | AAAA |
| ATOM | 124 | CB | TYR | 17 | 30.662 | 39.306 | 42.672 | 1.00 | 41.05 | AAAA |
| ATOM | 125 | CG | TYR | 17 | 31.040 | 38.104 | 43.519 | 1.00 | 37.51 | AAAA |
| ATOM | 126 | CD1 | TYR | 17 | 32.039 | 38.194 | 44.493 | 1.00 | 32.59 | AAAA |
| ATOM | 127 | CE1 | TYR | 17 | 32.383 | 37.095 | 45.277 | 1.00 | 29.32 | AAAA |
| ATOM | 128 | CD2 | TYR | 17 | 30.393 | 36.875 | 43.346 | 1.00 | 31.46 | AAAA |
| ATOM | 129 | CE2 | TYR | 17 | 30.726 | 35.772 | 44.122 | 1.00 | 28.64 | AAAA |
| ATOM | 130 | CZ | TYR | 17 | 31.721 | 35.887 | 45.088 | 1.00 | 27.14 | AAAA |
| ATOM | 131 | OH | TYR | 17 | 32.044 | 34.807 | 45.881 | 1.00 | 21.73 | AAAA |
| ATOM | 132 | C | TYR | 17 | 31.380 | 40.871 | 40.836 | 1.00 | 40.97 | AAAA |

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Figure 16-3

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 133 | O | TYR | 17 | 31.435 | 42.097 | 40.984 | 1.00 | 29.58 | AAAA |
| ATOM | 134 | N | PRO | 18 | 30.904 | 40.321 | 39.722 | 1.00 | 41.02 | AAAA |
| ATOM | 135 | CD | PRO | 18 | 30.760 | 38.910 | 39.318 | 1.00 | 48.67 | AAAA |
| ATOM | 136 | CA | PRO | 18 | 30.459 | 41.197 | 38.649 | 1.00 | 49.35 | AAAA |
| ATOM | 137 | CB | PRO | 18 | 30.321 | 40.228 | 37.481 | 1.00 | 59.04 | AAAA |
| ATOM | 138 | CG | PRO | 18 | 29.756 | 39.017 | 38.179 | 1.00 | 54.15 | AAAA |
| ATOM | 139 | C | PRO | 18 | 29.178 | 41.982 | 38.864 | 1.00 | 54.97 | AAAA |
| ATOM | 140 | O | PRO | 18 | 28.457 | 41.823 | 39.850 | 1.00 | 46.85 | AAAA |
| ATOM | 141 | N | LYS | 19 | 28.961 | 42.868 | 37.904 | 1.00 | 60.87 | AAAA |
| ATOM | 142 | CA | LYS | 19 | 27.777 | 43.696 | 37.749 | 1.00 | 67.78 | AAAA |
| ATOM | 143 | CB | LYS | 19 | 27.155 | 43.278 | 36.425 | 1.00 | 73.26 | AAAA |
| ATOM | 144 | CG | LYS | 19 | 26.971 | 41.752 | 36.414 | 1.00 | 77.87 | AAAA |
| ATOM | 145 | CD | LYS | 19 | 26.276 | 41.166 | 35.209 | 1.00 | 81.01 | AAAA |
| ATOM | 146 | CE | LYS | 19 | 26.039 | 39.680 | 35.471 | 1.00 | 82.45 | AAAA |
| ATOM | 147 | NZ | LYS | 19 | 25.417 | 38.959 | 34.331 | 1.00 | 83.11 | AAAA |
| ATOM | 148 | C | LYS | 19 | 26.688 | 43.594 | 38.814 | 1.00 | 64.15 | AAAA |
| ATOM | 149 | O | LYS | 19 | 26.810 | 44.047 | 39.949 | 1.00 | 65.73 | AAAA |
| ATOM | 150 | N | ASN | 20 | 25.604 | 42.986 | 38.345 | 1.00 | 59.78 | AAAA |
| ATOM | 151 | CA | ASN | 20 | 24.353 | 42.703 | 39.025 | 1.00 | 59.91 | AAAA |
| ATOM | 152 | CB | ASN | 20 | 23.516 | 41.844 | 38.077 | 1.00 | 68.08 | AAAA |
| ATOM | 153 | CG | ASN | 20 | 22.108 | 42.355 | 37.907 | 1.00 | 78.73 | AAAA |
| ATOM | 154 | OD1 | ASN | 20 | 21.894 | 43.498 | 37.496 | 1.00 | 78.67 | AAAA |
| ATOM | 155 | ND2 | ASN | 20 | 21.132 | 41.505 | 38.211 | 1.00 | 83.22 | AAAA |
| ATOM | 156 | C | ASN | 20 | 24.474 | 41.977 | 40.361 | 1.00 | 53.35 | AAAA |
| ATOM | 157 | O | ASN | 20 | 23.611 | 42.112 | 41.234 | 1.00 | 59.92 | AAAA |
| ATOM | 158 | N | HIS | 21 | 25.543 | 41.206 | 40.511 | 1.00 | 44.23 | AAAA |
| ATOM | 159 | CA | HIS | 21 | 25.768 | 40.397 | 41.707 | 1.00 | 28.15 | AAAA |
| ATOM | 160 | CB | HIS | 21 | 27.088 | 39.639 | 41.570 | 1.00 | 31.84 | AAAA |
| ATOM | 161 | CG | HIS | 21 | 27.155 | 38.411 | 42.418 | 1.00 | 34.79 | AAAA |
| ATOM | 162 | CD2 | HIS | 21 | 27.344 | 38.259 | 43.752 | 1.00 | 25.03 | AAAA |
| ATOM | 163 | ND1 | HIS | 21 | 26.929 | 37.148 | 41.917 | 1.00 | 34.81 | AAAA |
| ATOM | 164 | CE1 | HIS | 21 | 26.979 | 36.269 | 42.900 | 1.00 | 17.01 | AAAA |
| ATOM | 165 | NE2 | HIS | 21 | 27.228 | 36.917 | 44.026 | 1.00 | 32.31 | AAAA |
| ATOM | 166 | C | HIS | 21 | 25.763 | 41.135 | 43.051 | 1.00 | 29.37 | AAAA |
| ATOM | 167 | O | HIS | 21 | 26.346 | 42.210 | 43.186 | 1.00 | 28.54 | AAAA |
| ATOM | 168 | N | PRO | 22 | 25.093 | 40.565 | 44.066 | 1.00 | 29.14 | AAAA |
| ATOM | 169 | CD | PRO | 22 | 24.301 | 39.322 | 44.061 | 1.00 | 31.20 | AAAA |
| ATOM | 170 | CA | PRO | 22 | 25.034 | 41.185 | 45.395 | 1.00 | 32.84 | AAAA |
| ATOM | 171 | CB | PRO | 22 | 24.174 | 40.192 | 46.187 | 1.00 | 34.98 | AAAA |
| ATOM | 172 | CG | PRO | 22 | 23.257 | 39.634 | 45.109 | 1.00 | 30.11 | AAAA |
| ATOM | 173 | C | PRO | 22 | 26.411 | 41.415 | 46.044 | 1.00 | 34.37 | AAAA |
| ATOM | 174 | O | PRO | 22 | 26.554 | 42.272 | 46.916 | 1.00 | 29.17 | AAAA |
| ATOM | 175 | N | LEU | 23 | 27.415 | 40.644 | 45.629 | 1.00 | 29.22 | AAAA |
| ATOM | 176 | CA | LEU | 23 | 28.765 | 40.781 | 46.181 | 1.00 | 26.49 | AAAA |
| ATOM | 177 | CB | LEU | 23 | 29.414 | 39.397 | 46.332 | 1.00 | 22.30 | AAAA |
| ATOM | 178 | CG | LEU | 23 | 28.703 | 38.527 | 47.380 | 1.00 | 21.04 | AAAA |
| ATOM | 179 | CD1 | LEU | 23 | 29.307 | 37.113 | 47.410 | 1.00 | 19.35 | AAAA |
| ATOM | 180 | CD2 | LEU | 23 | 28.850 | 39.197 | 48.746 | 1.00 | 26.51 | AAAA |
| ATOM | 181 | C | LEU | 23 | 29.661 | 41.718 | 45.361 | 1.00 | 25.81 | AAAA |
| ATOM | 182 | O | LEU | 23 | 30.893 | 41.693 | 45.477 | 1.00 | 28.45 | AAAA |
| ATOM | 183 | N | LYS | 24 | 29.018 | 42.539 | 44.532 | 1.00 | 24.86 | AAAA |
| ATOM | 184 | CA | LYS | 24 | 29.696 | 43.552 | 43.723 | 1.00 | 27.35 | AAAA |
| ATOM | 185 | CB | LYS | 24 | 28.662 | 44.244 | 42.830 | 1.00 | 28.57 | AAAA |
| ATOM | 186 | CG | LYS | 24 | 29.118 | 45.532 | 42.171 | 1.00 | 52.95 | AAAA |
| ATOM | 187 | CD | LYS | 24 | 28.025 | 46.603 | 42.283 | 1.00 | 63.74 | AAAA |
| ATOM | 188 | CE | LYS | 24 | 26.688 | 46.138 | 41.706 | 1.00 | 66.09 | AAAA |
| ATOM | 189 | NZ | LYS | 24 | 25.595 | 47.137 | 41.896 | 1.00 | 66.00 | AAAA |
| ATOM | 190 | C | LYS | 24 | 30.332 | 44.592 | 44.676 | 1.00 | 29.52 | AAAA |
| ATOM | 191 | O | LYS | 24 | 31.412 | 45.123 | 44.420 | 1.00 | 30.67 | AAAA |
| ATOM | 192 | N | ILE | 25 | 29.652 | 44.879 | 45.779 | 1.00 | 26.90 | AAAA |
| ATOM | 193 | CA | ILE | 25 | 30.151 | 45.865 | 46.738 | 1.00 | 25.02 | AAAA |
| ATOM | 194 | CB | ILE | 25 | 29.105 | 46.177 | 47.824 | 1.00 | 28.34 | AAAA |
| ATOM | 195 | CG2 | ILE | 25 | 27.961 | 46.951 | 47.237 | 1.00 | 23.84 | AAAA |
| ATOM | 196 | CG1 | ILE | 25 | 28.661 | 44.869 | 48.495 | 1.00 | 30.31 | AAAA |
| ATOM | 197 | CD1 | ILE | 25 | 27.718 | 45.051 | 49.660 | 1.00 | 44.90 | AAAA |
| ATOM | 198 | C | ILE | 25 | 31.424 | 45.463 | 47.483 | 1.00 | 32.19 | AAAA |

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Figure 16-4

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 199 | O | ILE | 25 | 31.736 | 44.271 | 47.623 | 1.00 | 26.54 | AAAA |
| ATOM | 200 | N | PRO | 26 | 32.191 | 46.463 | 47.956 | 1.00 | 30.14 | AAAA |
| ATOM | 201 | CD | PRO | 26 | 31.979 | 47.907 | 47.770 | 1.00 | 36.38 | AAAA |
| ATOM | 202 | CA | PRO | 26 | 33.431 | 46.241 | 48.707 | 1.00 | 30.63 | AAAA |
| ATOM | 203 | CB | PRO | 26 | 34.014 | 47.652 | 48.814 | 1.00 | 34.29 | AAAA |
| ATOM | 204 | CG | PRO | 26 | 33.397 | 48.373 | 47.617 | 1.00 | 43.39 | AAAA |
| ATOM | 205 | C | PRO | 26 | 32.943 | 45.727 | 50.061 | 1.00 | 25.99 | AAAA |
| ATOM | 206 | O | PRO | 26 | 31.854 | 46.110 | 50.484 | 1.00 | 25.51 | AAAA |
| ATOM | 207 | N | ARG | 27 | 33.719 | 44.880 | 50.743 | 1.00 | 21.98 | AAAA |
| ATOM | 208 | CA | ARG | 27 | 33.267 | 44.347 | 52.035 | 1.00 | 26.17 | AAAA |
| ATOM | 209 | CB | ARG | 27 | 32.641 | 42.969 | 51.834 | 1.00 | 22.70 | AAAA |
| ATOM | 210 | CG | ARG | 27 | 31.442 | 43.039 | 50.890 | 1.00 | 26.75 | AAAA |
| ATOM | 211 | CD | ARG | 27 | 30.832 | 41.672 | 50.581 | 1.00 | 33.22 | AAAA |
| ATOM | 212 | NE | ARG | 27 | 30.121 | 41.098 | 51.716 | 1.00 | 28.66 | AAAA |
| ATOM | 213 | CZ | ARG | 27 | 30.582 | 40.129 | 52.503 | 1.00 | 31.79 | AAAA |
| ATOM | 214 | NH1 | ARG | 27 | 31.778 | 39.598 | 52.290 | 1.00 | 34.08 | AAAA |
| ATOM | 215 | NH2 | ARG | 27 | 29.833 | 39.688 | 53.505 | 1.00 | 26.16 | AAAA |
| ATOM | 216 | C | ARG | 27 | 34.358 | 44.297 | 53.090 | 1.00 | 24.10 | AAAA |
| ATOM | 217 | O | ARG | 27 | 34.326 | 45.074 | 54.038 | 1.00 | 23.50 | AAAA |
| ATOM | 218 | N | VAL | 28 | 35.314 | 43.390 | 52.960 | 1.00 | 21.45 | AAAA |
| ATOM | 219 | CA | VAL | 28 | 36.385 | 43.385 | 53.953 | 1.00 | 21.75 | AAAA |
| ATOM | 220 | CB | VAL | 28 | 37.221 | 42.101 | 53.866 | 1.00 | 26.55 | AAAA |
| ATOM | 221 | CG1 | VAL | 28 | 38.407 | 42.177 | 54.830 | 1.00 | 23.84 | AAAA |
| ATOM | 222 | CG2 | VAL | 28 | 36.337 | 40.906 | 54.214 | 1.00 | 19.20 | AAAA |
| ATOM | 223 | C | VAL | 28 | 37.277 | 44.611 | 53.736 | 1.00 | 20.86 | AAAA |
| ATOM | 224 | O | VAL | 28 | 37.770 | 45.223 | 54.702 | 1.00 | 25.15 | AAAA |
| ATOM | 225 | N | SER | 29 | 37.480 | 44.996 | 52.475 | 1.00 | 19.22 | AAAA |
| ATOM | 226 | CA | SER | 29 | 38.320 | 46.169 | 52.209 | 1.00 | 19.63 | AAAA |
| ATOM | 227 | CB | SER | 29 | 38.591 | 46.352 | 50.702 | 1.00 | 24.45 | AAAA |
| ATOM | 228 | CG | SER | 29 | 37.411 | 46.697 | 49.984 | 1.00 | 28.74 | AAAA |
| ATOM | 229 | C | SER | 29 | 37.579 | 47.381 | 52.756 | 1.00 | 21.50 | AAAA |
| ATOM | 230 | O | SER | 29 | 38.184 | 48.320 | 53.271 | 1.00 | 18.95 | AAAA |
| ATOM | 231 | N | LEU | 30 | 36.256 | 47.353 | 52.673 | 1.00 | 19.56 | AAAA |
| ATOM | 232 | CA | LEU | 30 | 35.499 | 48.481 | 53.177 | 1.00 | 25.97 | AAAA |
| ATOM | 233 | CB | LEU | 30 | 34.032 | 48.396 | 52.744 | 1.00 | 22.90 | AAAA |
| ATOM | 234 | CG | LEU | 30 | 33.085 | 49.541 | 53.157 | 1.00 | 26.62 | AAAA |
| ATOM | 235 | CD1 | LEU | 30 | 32.885 | 49.539 | 54.648 | 1.00 | 38.27 | AAAA |
| ATOM | 236 | CD2 | LEU | 30 | 33.653 | 50.885 | 52.698 | 1.00 | 25.71 | AAAA |
| ATOM | 237 | C | LEU | 30 | 35.604 | 48.509 | 54.696 | 1.00 | 18.44 | AAAA |
| ATOM | 238 | O | LEU | 30 | 35.704 | 49.580 | 55.273 | 1.00 | 25.05 | AAAA |
| ATOM | 239 | N | LEU | 31 | 35.578 | 47.336 | 55.336 | 1.00 | 19.65 | AAAA |
| ATOM | 240 | CA | LEU | 31 | 35.672 | 47.270 | 56.797 | 1.00 | 20.47 | AAAA |
| ATOM | 241 | CB | LEU | 31 | 35.613 | 45.821 | 57.300 | 1.00 | 20.60 | AAAA |
| ATOM | 242 | CG | LEU | 31 | 34.988 | 45.456 | 58.665 | 1.00 | 39.80 | AAAA |
| ATOM | 243 | CD1 | LEU | 31 | 35.712 | 44.219 | 59.257 | 1.00 | 23.99 | AAAA |
| ATOM | 244 | CD2 | LEU | 31 | 35.085 | 46.591 | 59.637 | 1.00 | 28.48 | AAAA |
| ATOM | 245 | C | LEU | 31 | 37.009 | 47.870 | 57.229 | 1.00 | 23.85 | AAAA |
| ATOM | 246 | O | LEU | 31 | 37.070 | 48.673 | 58.154 | 1.00 | 21.24 | AAAA |
| ATOM | 247 | N | LEU | 32 | 38.079 | 47.462 | 56.562 | 1.00 | 23.91 | AAAA |
| ATOM | 248 | CA | LEU | 32 | 39.400 | 47.965 | 56.899 | 1.00 | 24.82 | AAAA |
| ATOM | 249 | CB | LEU | 32 | 40.479 | 47.320 | 56.018 | 1.00 | 24.81 | AAAA |
| ATOM | 250 | CG | LEU | 32 | 40.849 | 45.854 | 56.276 | 1.00 | 27.00 | AAAA |
| ATOM | 251 | CD1 | LEU | 32 | 41.995 | 45.435 | 55.354 | 1.00 | 27.13 | AAAA |
| ATOM | 252 | CD2 | LEU | 32 | 41.285 | 45.687 | 57.720 | 1.00 | 34.49 | AAAA |
| ATOM | 253 | C | LEU | 32 | 39.466 | 49.475 | 56.763 | 1.00 | 19.56 | AAAA |
| ATOM | 254 | O | LEU | 32 | 39.958 | 50.143 | 57.662 | 1.00 | 20.71 | AAAA |
| ATOM | 255 | N | ARG | 33 | 38.974 | 50.006 | 55.645 | 1.00 | 23.25 | AAAA |
| ATOM | 256 | CA | ARG | 33 | 39.007 | 51.449 | 55.441 | 1.00 | 24.33 | AAAA |
| ATOM | 257 | CB | ARG | 33 | 38.575 | 51.806 | 54.013 | 1.00 | 23.46 | AAAA |
| ATOM | 258 | CG | ARG | 33 | 39.571 | 51.327 | 52.945 | 1.00 | 26.94 | AAAA |
| ATOM | 259 | CD | ARG | 33 | 39.337 | 51.976 | 51.585 | 1.00 | 42.13 | AAAA |
| ATOM | 260 | NE | ARG | 33 | 38.023 | 51.661 | 51.037 | 1.00 | 59.06 | AAAA |
| ATOM | 261 | CZ | ARG | 33 | 37.583 | 52.088 | 49.857 | 1.00 | 60.87 | AAAA |
| ATOM | 262 | NH1 | ARG | 33 | 38.353 | 52.850 | 49.095 | 1.00 | 65.33 | AAAA |
| ATOM | 263 | NH2 | ARG | 33 | 36.373 | 51.743 | 49.433 | 1.00 | 56.24 | AAAA |
| ATOM | 264 | C | ARG | 33 | 38.124 | 52.156 | 56.455 | 1.00 | 30.33 | AAAA |

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Figure 16-5

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 265 | O | ARG | 33 | 38.441 | 53.252 | 56.905 | 1.00 | 25.45 | AAAA |
| ATOM | 266 | N | PHE | 34 | 37.022 | 51.514 | 56.828 | 1.00 | 24.98 | AAAA |
| ATOM | 267 | CA | PHE | 34 | 36.099 | 52.085 | 57.789 | 1.00 | 27.09 | AAAA |
| ATOM | 268 | CB | PHE | 34 | 34.798 | 51.276 | 57.807 | 1.00 | 24.88 | AAAA |
| ATOM | 269 | CG | PHE | 34 | 33.719 | 51.898 | 58.631 | 1.00 | 20.46 | AAAA |
| ATOM | 270 | CD1 | PHE | 34 | 33.043 | 53.018 | 58.171 | 1.00 | 18.74 | AAAA |
| ATOM | 271 | CD2 | PHE | 34 | 33.396 | 51.383 | 59.889 | 1.00 | 20.19 | AAAA |
| ATOM | 272 | CE1 | PHE | 34 | 32.043 | 53.627 | 58.956 | 1.00 | 23.04 | AAAA |
| ATOM | 273 | CE2 | PHE | 34 | 32.406 | 51.974 | 60.681 | 1.00 | 25.08 | AAAA |
| ATOM | 274 | CZ | PHE | 34 | 31.726 | 53.104 | 60.209 | 1.00 | 23.31 | AAAA |
| ATOM | 275 | C | PHE | 34 | 36.709 | 52.115 | 59.194 | 1.00 | 23.93 | AAAA |
| ATOM | 276 | O | PHE | 34 | 36.668 | 53.138 | 59.883 | 1.00 | 21.71 | AAAA |
| ATOM | 277 | N | LYS | 35 | 37.298 | 51.013 | 59.645 | 1.00 | 21.33 | AAAA |
| ATOM | 278 | CA | LYS | 35 | 37.862 | 51.084 | 60.978 | 1.00 | 22.54 | AAAA |
| ATOM | 279 | CB | LYS | 35 | 38.276 | 49.716 | 61.476 | 1.00 | 29.70 | AAAA |
| ATOM | 280 | CG | LYS | 35 | 37.082 | 48.890 | 61.924 | 1.00 | 29.48 | AAAA |
| ATOM | 281 | CD | LYS | 35 | 37.517 | 47.535 | 62.398 | 1.00 | 42.17 | AAAA |
| ATOM | 282 | CE | LYS | 35 | 38.157 | 46.762 | 61.275 | 1.00 | 34.89 | AAAA |
| ATOM | 283 | NZ | LYS | 35 | 39.372 | 47.412 | 60.719 | 1.00 | 67.18 | AAAA |
| ATOM | 284 | C | LYS | 35 | 39.027 | 52.055 | 61.040 | 1.00 | 24.68 | AAAA |
| ATOM | 285 | O | LYS | 35 | 39.282 | 52.640 | 62.085 | 1.00 | 22.33 | AAAA |
| ATOM | 286 | N | ASP | 36 | 39.724 | 52.231 | 59.926 | 1.00 | 25.67 | AAAA |
| ATOM | 287 | CA | ASP | 36 | 40.842 | 53.163 | 59.898 | 1.00 | 25.57 | AAAA |
| ATOM | 288 | CB | ASP | 36 | 41.669 | 52.984 | 58.621 | 1.00 | 32.26 | AAAA |
| ATOM | 289 | CG | ASP | 36 | 42.881 | 53.914 | 58.572 | 1.00 | 33.92 | AAAA |
| ATOM | 290 | OD1 | ASP | 36 | 43.641 | 53.969 | 59.563 | 1.00 | 40.22 | AAAA |
| ATOM | 291 | OD2 | ASP | 36 | 43.078 | 54.575 | 57.538 | 1.00 | 40.06 | AAAA |
| ATOM | 292 | C | ASP | 36 | 40.285 | 54.578 | 59.973 | 1.00 | 28.04 | AAAA |
| ATOM | 293 | O | ASP | 36 | 40.761 | 55.397 | 60.765 | 1.00 | 29.52 | AAAA |
| ATOM | 294 | N | ALA | 37 | 39.272 | 54.864 | 59.159 | 1.00 | 23.32 | AAAA |
| ATOM | 295 | CA | ALA | 37 | 38.651 | 56.192 | 59.163 | 1.00 | 28.22 | AAAA |
| ATOM | 296 | CB | ALA | 37 | 37.506 | 56.251 | 58.119 | 1.00 | 25.93 | AAAA |
| ATOM | 297 | C | ALA | 37 | 38.127 | 56.549 | 60.565 | 1.00 | 28.41 | AAAA |
| ATOM | 298 | O | ALA | 37 | 38.186 | 57.708 | 60.972 | 1.00 | 29.27 | AAAA |
| ATOM | 299 | N | MET | 38 | 37.639 | 55.547 | 61.300 | 1.00 | 24.76 | AAAA |
| ATOM | 300 | CA | MET | 38 | 37.103 | 55.727 | 62.669 | 1.00 | 25.45 | AAAA |
| ATOM | 301 | CB | MET | 38 | 36.077 | 54.625 | 62.982 | 1.00 | 25.19 | AAAA |
| ATOM | 302 | CG | MET | 38 | 34.816 | 54.660 | 62.148 | 1.00 | 22.32 | AAAA |
| ATOM | 303 | SD | MET | 38 | 33.733 | 55.983 | 62.702 | 1.00 | 29.90 | AAAA |
| ATOM | 304 | CE | MET | 38 | 33.402 | 55.417 | 64.376 | 1.00 | 26.51 | AAAA |
| ATOM | 305 | C | MET | 38 | 38.203 | 55.667 | 63.744 | 1.00 | 26.42 | AAAA |
| ATOM | 306 | O | MET | 38 | 37.924 | 55.818 | 64.947 | 1.00 | 23.77 | AAAA |
| ATOM | 307 | N | ASN | 39 | 39.437 | 55.434 | 63.300 | 1.00 | 26.21 | AAAA |
| ATOM | 308 | CA | ASN | 39 | 40.607 | 55.308 | 64.170 | 1.00 | 28.53 | AAAA |
| ATOM | 309 | CB | ASN | 39 | 40.926 | 56.643 | 64.855 | 1.00 | 33.95 | AAAA |
| ATOM | 310 | CG | ASN | 39 | 41.153 | 57.751 | 63.858 | 1.00 | 29.46 | AAAA |
| ATOM | 311 | OD1 | ASN | 39 | 41.930 | 57.596 | 62.925 | 1.00 | 36.28 | AAAA |
| ATOM | 312 | ND2 | ASN | 39 | 40.472 | 58.880 | 64.046 | 1.00 | 40.03 | AAAA |
| ATOM | 313 | C | ASN | 39 | 40.374 | 54.223 | 65.205 | 1.00 | 30.07 | AAAA |
| ATOM | 314 | O | ASN | 39 | 40.682 | 54.390 | 66.395 | 1.00 | 25.47 | AAAA |
| ATOM | 315 | N | LEU | 40 | 39.814 | 53.105 | 64.744 | 1.00 | 28.19 | AAAA |
| ATOM | 316 | CA | LEU | 40 | 39.527 | 51.984 | 65.633 | 1.00 | 25.50 | AAAA |
| ATOM | 317 | CB | LEU | 40 | 38.060 | 51.562 | 65.514 | 1.00 | 32.14 | AAAA |
| ATOM | 318 | CG | LEU | 40 | 37.044 | 52.585 | 66.036 | 1.00 | 30.47 | AAAA |
| ATOM | 319 | CD1 | LEU | 40 | 35.637 | 52.027 | 65.894 | 1.00 | 29.07 | AAAA |
| ATOM | 320 | CD2 | LEU | 40 | 37.325 | 52.889 | 67.491 | 1.00 | 23.80 | AAAA |
| ATOM | 321 | C | LEU | 40 | 40.433 | 50.771 | 65.415 | 1.00 | 26.99 | AAAA |
| ATOM | 322 | O | LEU | 40 | 40.157 | 49.683 | 65.915 | 1.00 | 25.41 | AAAA |
| ATOM | 323 | N | ILE | 41 | 41.528 | 50.970 | 64.691 | 1.00 | 28.33 | AAAA |
| ATOM | 324 | CA | ILE | 41 | 42.459 | 49.882 | 64.459 | 1.00 | 25.08 | AAAA |
| ATOM | 325 | CB | ILE | 41 | 42.010 | 49.020 | 63.243 | 1.00 | 25.01 | AAAA |
| ATOM | 326 | CG2 | ILE | 41 | 42.061 | 49.824 | 61.961 | 1.00 | 22.74 | AAAA |
| ATOM | 327 | CG1 | ILE | 41 | 42.917 | 47.802 | 63.128 | 1.00 | 31.01 | AAAA |
| ATOM | 328 | CD1 | ILE | 41 | 42.895 | 46.951 | 64.341 | 1.00 | 42.18 | AAAA |
| ATOM | 329 | C | ILE | 41 | 43.900 | 50.376 | 64.247 | 1.00 | 24.09 | AAAA |
| ATOM | 330 | O | ILE | 41 | 44.128 | 51.406 | 63.621 | 1.00 | 28.92 | AAAA |

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Figure 16-6

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 331 | N | ASP | 42 | 44.866 | 49.634 | 64.787 | 1.00 | 28.95 | AAAA |
| ATOM | 332 | CA | ASP | 42 | 46.279 | 49.988 | 64.638 | 1.00 | 32.52 | AAAA |
| ATOM | 333 | CB | ASP | 42 | 46.951 | 50.094 | 66.007 | 1.00 | 34.24 | AAAA |
| ATOM | 334 | CG | ASP | 42 | 46.267 | 51.097 | 66.911 | 1.00 | 51.23 | AAAA |
| ATOM | 335 | OD1 | ASP | 42 | 46.079 | 52.250 | 66.467 | 1.00 | 50.19 | AAAA |
| ATOM | 336 | OD2 | ASP | 42 | 45.924 | 50.736 | 68.062 | 1.00 | 53.00 | AAAA |
| ATOM | 337 | C | ASP | 42 | 46.985 | 48.919 | 63.808 | 1.00 | 31.13 | AAAA |
| ATOM | 338 | O | ASP | 42 | 46.594 | 47.758 | 63.838 | 1.00 | 26.71 | AAAA |
| ATOM | 339 | N | GLU | 43 | 48.036 | 49.312 | 63.092 | 1.00 | 29.99 | AAAA |
| ATOM | 340 | CA | GLU | 43 | 48.793 | 48.392 | 62.240 | 1.00 | 31.34 | AAAA |
| ATOM | 341 | CB | GLU | 43 | 50.078 | 49.045 | 61.724 | 1.00 | 36.12 | AAAA |
| ATOM | 342 | CG | GLU | 43 | 49.886 | 50.118 | 60.676 | 1.00 | 52.72 | AAAA |
| ATOM | 343 | CD | GLU | 43 | 51.214 | 50.556 | 60.083 | 1.00 | 60.39 | AAAA |
| ATOM | 344 | OE1 | GLU | 43 | 51.928 | 49.688 | 59.536 | 1.00 | 70.32 | AAAA |
| ATOM | 345 | OE2 | GLU | 43 | 51.550 | 51.755 | 60.163 | 1.00 | 60.38 | AAAA |
| ATOM | 346 | C | GLU | 43 | 49.196 | 47.070 | 62.859 | 1.00 | 38.04 | AAAA |
| ATOM | 347 | O | GLU | 43 | 49.125 | 46.024 | 62.209 | 1.00 | 36.83 | AAAA |
| ATOM | 348 | N | LYS | 44 | 49.636 | 47.103 | 64.105 | 1.00 | 28.26 | AAAA |
| ATOM | 349 | CA | LYS | 44 | 50.084 | 45.879 | 64.740 | 1.00 | 32.71 | AAAA |
| ATOM | 350 | CB | LYS | 44 | 50.974 | 46.245 | 65.927 | 1.00 | 44.28 | AAAA |
| ATOM | 351 | CG | LYS | 44 | 52.211 | 47.007 | 65.418 | 1.00 | 59.37 | AAAA |
| ATOM | 352 | CD | LYS | 44 | 53.187 | 47.449 | 66.491 | 1.00 | 68.87 | AAAA |
| ATOM | 353 | CE | LYS | 44 | 54.373 | 48.167 | 65.849 | 1.00 | 67.21 | AAAA |
| ATOM | 354 | NZ | LYS | 44 | 55.361 | 48.648 | 66.850 | 1.00 | 74.00 | AAAA |
| ATOM | 355 | C | LYS | 44 | 48.982 | 44.889 | 65.115 | 1.00 | 26.75 | AAAA |
| ATOM | 356 | O | LYS | 44 | 49.265 | 43.792 | 65.586 | 1.00 | 27.37 | AAAA |
| ATOM | 357 | N | GLU | 45 | 47.731 | 45.278 | 64.881 | 1.00 | 29.20 | AAAA |
| ATOM | 358 | CA | GLU | 45 | 46.580 | 44.414 | 65.165 | 1.00 | 21.58 | AAAA |
| ATOM | 359 | CB | GLU | 45 | 45.387 | 45.243 | 65.676 | 1.00 | 18.24 | AAAA |
| ATOM | 360 | CG | GLU | 45 | 45.551 | 45.828 | 67.077 | 1.00 | 26.57 | AAAA |
| ATOM | 361 | CD | GLU | 45 | 44.418 | 46.772 | 67.453 | 1.00 | 23.12 | AAAA |
| ATOM | 362 | OE1 | GLU | 45 | 44.224 | 47.783 | 66.746 | 1.00 | 21.64 | AAAA |
| ATOM | 363 | OE2 | GLU | 45 | 43.725 | 46.509 | 68.454 | 1.00 | 26.48 | AAAA |
| ATOM | 364 | C | GLU | 45 | 46.163 | 43.710 | 63.870 | 1.00 | 26.31 | AAAA |
| ATOM | 365 | O | GLU | 45 | 45.400 | 42.739 | 63.889 | 1.00 | 22.32 | AAAA |
| ATOM | 366 | N | LEU | 46 | 46.674 | 44.204 | 62.748 | 1.00 | 20.15 | AAAA |
| ATOM | 367 | CA | LEU | 46 | 46.317 | 43.642 | 61.448 | 1.00 | 25.80 | AAAA |
| ATOM | 368 | CB | LEU | 46 | 46.137 | 44.774 | 60.433 | 1.00 | 27.25 | AAAA |
| ATOM | 369 | CG | LEU | 46 | 45.763 | 44.397 | 58.997 | 1.00 | 37.72 | AAAA |
| ATOM | 370 | CD1 | LEU | 46 | 44.356 | 43.810 | 58.984 | 1.00 | 39.46 | AAAA |
| ATOM | 371 | CD2 | LEU | 46 | 45.822 | 45.632 | 58.101 | 1.00 | 35.43 | AAAA |
| ATOM | 372 | C | LEU | 46 | 47.305 | 42.623 | 60.896 | 1.00 | 28.88 | AAAA |
| ATOM | 373 | O | LEU | 46 | 48.513 | 42.860 | 60.862 | 1.00 | 31.98 | AAAA |
| ATOM | 374 | N | ILE | 47 | 46.791 | 41.469 | 60.482 | 1.00 | 16.92 | AAAA |
| ATOM | 375 | CA | ILE | 47 | 47.638 | 40.448 | 59.872 | 1.00 | 20.98 | AAAA |
| ATOM | 376 | CB | ILE | 47 | 47.412 | 39.046 | 60.513 | 1.00 | 21.51 | AAAA |
| ATOM | 377 | CG2 | ILE | 47 | 48.115 | 37.958 | 59.696 | 1.00 | 20.32 | AAAA |
| ATOM | 378 | CG1 | ILE | 47 | 47.947 | 39.040 | 60.950 | 1.00 | 20.71 | AAAA |
| ATOM | 379 | CD1 | ILE | 47 | 49.450 | 39.207 | 62.052 | 1.00 | 38.87 | AAAA |
| ATOM | 380 | C | ILE | 47 | 47.227 | 40.417 | 58.406 | 1.00 | 24.50 | AAAA |
| ATOM | 381 | O | ILE | 47 | 46.036 | 40.279 | 58.101 | 1.00 | 20.74 | AAAA |
| ATOM | 382 | N | LYS | 48 | 48.195 | 40.550 | 57.500 | 1.00 | 18.73 | AAAA |
| ATOM | 383 | CA | LYS | 48 | 47.883 | 40.543 | 56.072 | 1.00 | 15.55 | AAAA |
| ATOM | 384 | CB | LYS | 48 | 49.095 | 40.991 | 55.239 | 1.00 | 16.52 | AAAA |
| ATOM | 385 | CG | LYS | 48 | 48.836 | 41.011 | 53.738 | 1.00 | 23.25 | AAAA |
| ATOM | 386 | CD | LYS | 48 | 50.072 | 41.451 | 52.957 | 1.00 | 32.69 | AAAA |
| ATOM | 387 | CE | LYS | 48 | 49.796 | 41.496 | 51.462 | 1.00 | 26.00 | AAAA |
| ATOM | 388 | NZ | LYS | 48 | 48.704 | 42.449 | 51.114 | 1.00 | 46.33 | AAAA |
| ATOM | 389 | C | LYS | 48 | 47.473 | 39.140 | 55.629 | 1.00 | 14.43 | AAAA |
| ATOM | 390 | O | LYS | 48 | 48.177 | 38.174 | 55.887 | 1.00 | 16.83 | AAAA |
| ATOM | 391 | N | SER | 49 | 46.343 | 39.049 | 54.945 | 1.00 | 16.61 | AAAA |
| ATOM | 392 | CA | SER | 49 | 45.838 | 37.780 | 54.439 | 1.00 | 14.33 | AAAA |
| ATOM | 393 | CB | SER | 49 | 44.517 | 37.984 | 53.694 | 1.00 | 13.21 | AAAA |
| ATOM | 394 | OG | SER | 49 | 43.509 | 38.613 | 54.492 | 1.00 | 16.86 | AAAA |
| ATOM | 395 | C | SER | 49 | 46.810 | 37.131 | 53.459 | 1.00 | 24.11 | AAAA |
| ATOM | 396 | O | SER | 49 | 47.463 | 37.815 | 52.663 | 1.00 | 19.59 | AAAA |

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Figure 16-7

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 397 | N | ARG | 50 | 46.890 | 35.805 | 53.519 | 1.00 | 16.83 | AAAA |
| ATOM | 398 | CA | ARG | 50 | 47.724 | 35.037 | 52.610 | 1.00 | 23.88 | AAAA |
| ATOM | 399 | CB | ARG | 50 | 48.805 | 34.247 | 53.366 | 1.00 | 27.48 | AAAA |
| ATOM | 400 | CG | ARG | 50 | 48.284 | 33.036 | 54.177 | 1.00 | 22.99 | AAAA |
| ATOM | 401 | CD | ARG | 50 | 49.453 | 32.263 | 54.759 | 1.00 | 25.20 | AAAA |
| ATOM | 402 | NE | ARG | 50 | 49.073 | 31.197 | 55.684 | 1.00 | 15.88 | AAAA |
| ATOM | 403 | CZ | ARG | 50 | 48.411 | 30.093 | 55.368 | 1.00 | 14.34 | AAAA |
| ATOM | 404 | NH1 | ARG | 50 | 48.023 | 29.863 | 54.117 | 1.00 | 15.78 | AAAA |
| ATOM | 405 | NH2 | ARG | 50 | 48.150 | 29.197 | 56.312 | 1.00 | 16.78 | AAAA |
| ATOM | 406 | C | ARG | 50 | 46.821 | 34.023 | 51.905 | 1.00 | 20.20 | AAAA |
| ATOM | 407 | O | ARG | 50 | 45.763 | 33.650 | 52.414 | 1.00 | 18.63 | AAAA |
| ATOM | 408 | N | PRO | 51 | 47.203 | 33.596 | 50.699 | 1.00 | 15.63 | AAAA |
| ATOM | 409 | CD | PRO | 51 | 48.322 | 34.028 | 49.850 | 1.00 | 19.45 | AAAA |
| ATOM | 410 | CA | PRO | 51 | 46.387 | 32.606 | 49.994 | 1.00 | 14.35 | AAAA |
| ATOM | 411 | CB | PRO | 51 | 47.076 | 32.514 | 48.629 | 1.00 | 17.73 | AAAA |
| ATOM | 412 | CG | PRO | 51 | 47.707 | 33.890 | 48.475 | 1.00 | 17.62 | AAAA |
| ATOM | 413 | C | PRO | 51 | 46.452 | 31.256 | 50.708 | 1.00 | 15.73 | AAAA |
| ATOM | 414 | O | PRO | 51 | 47.460 | 30.942 | 51.350 | 1.00 | 18.67 | AAAA |
| ATOM | 415 | N | ALA | 52 | 45.377 | 30.470 | 50.618 | 1.00 | 11.47 | AAAA |
| ATOM | 416 | CA | ALA | 52 | 45.375 | 29.117 | 51.161 | 1.00 | 9.78 | AAAA |
| ATOM | 417 | CB | ALA | 52 | 43.967 | 28.529 | 51.112 | 1.00 | 12.19 | AAAA |
| ATOM | 418 | C | ALA | 52 | 46.301 | 28.342 | 50.209 | 1.00 | 17.19 | AAAA |
| ATOM | 419 | O | ALA | 52 | 46.307 | 28.609 | 49.006 | 1.00 | 16.46 | AAAA |
| ATOM | 420 | N | THR | 53 | 47.081 | 27.392 | 50.723 | 1.00 | 16.40 | AAAA |
| ATOM | 421 | CA | THR | 53 | 47.952 | 26.615 | 49.843 | 1.00 | 16.32 | AAAA |
| ATOM | 422 | CB | THR | 53 | 49.109 | 25.959 | 50.612 | 1.00 | 15.82 | AAAA |
| ATOM | 423 | OG1 | THR | 53 | 48.582 | 25.016 | 51.559 | 1.00 | 16.25 | AAAA |
| ATOM | 424 | CG2 | THR | 53 | 49.923 | 27.030 | 51.336 | 1.00 | 14.34 | AAAA |
| ATOM | 425 | C | THR | 53 | 47.104 | 25.520 | 49.215 | 1.00 | 14.06 | AAAA |
| ATOM | 426 | O | THR | 53 | 46.012 | 25.241 | 49.690 | 1.00 | 17.87 | AAAA |
| ATOM | 427 | N | LYS | 54 | 47.599 | 24.903 | 48.145 | 1.00 | 16.10 | AAAA |
| ATOM | 428 | CA | LYS | 54 | 46.848 | 23.832 | 47.492 | 1.00 | 19.00 | AAAA |
| ATOM | 429 | CB | LYS | 54 | 47.671 | 23.245 | 46.339 | 1.00 | 22.92 | AAAA |
| ATOM | 430 | CG | LYS | 54 | 46.955 | 22.172 | 45.539 | 1.00 | 32.99 | AAAA |
| ATOM | 431 | CD | LYS | 54 | 45.787 | 22.733 | 44.757 | 1.00 | 51.34 | AAAA |
| ATOM | 432 | CE | LYS | 54 | 46.244 | 23.565 | 43.561 | 1.00 | 64.17 | AAAA |
| ATOM | 433 | NZ | LYS | 54 | 46.898 | 22.733 | 42.505 | 1.00 | 63.45 | AAAA |
| ATOM | 434 | C | LYS | 54 | 46.554 | 22.738 | 48.520 | 1.00 | 22.48 | AAAA |
| ATOM | 435 | O | LYS | 54 | 45.463 | 22.158 | 48.555 | 1.00 | 19.97 | AAAA |
| ATOM | 436 | N | GLU | 55 | 47.536 | 22.465 | 49.364 | 1.00 | 25.65 | AAAA |
| ATOM | 437 | CA | GLU | 55 | 47.389 | 21.432 | 50.383 | 1.00 | 25.08 | AAAA |
| ATOM | 438 | CB | GLU | 55 | 48.718 | 21.241 | 51.116 | 1.00 | 25.40 | AAAA |
| ATOM | 439 | CG | GLU | 55 | 48.703 | 20.185 | 52.199 | 1.00 | 48.95 | AAAA |
| ATOM | 440 | CD | GLU | 55 | 50.106 | 19.821 | 52.673 | 1.00 | 64.21 | AAAA |
| ATOM | 441 | OE1 | GLU | 55 | 50.220 | 19.033 | 53.640 | 1.00 | 62.38 | AAAA |
| ATOM | 442 | OE2 | GLU | 55 | 51.093 | 20.311 | 52.073 | 1.00 | 58.22 | AAAA |
| ATOM | 443 | C | GLU | 55 | 46.273 | 21.773 | 51.362 | 1.00 | 18.91 | AAAA |
| ATOM | 444 | O | GLU | 55 | 45.489 | 20.908 | 51.723 | 1.00 | 17.43 | AAAA |
| ATOM | 445 | N | GLU | 56 | 46.196 | 23.029 | 51.786 | 1.00 | 16.80 | AAAA |
| ATOM | 446 | CA | GLU | 56 | 45.137 | 23.432 | 52.698 | 1.00 | 17.24 | AAAA |
| ATOM | 447 | CB | GLU | 56 | 45.399 | 24.855 | 53.204 | 1.00 | 16.15 | AAAA |
| ATOM | 448 | CG | GLU | 56 | 46.709 | 24.941 | 54.009 | 1.00 | 14.41 | AAAA |
| ATOM | 449 | CD | GLU | 56 | 47.087 | 26.354 | 54.358 | 1.00 | 20.17 | AAAA |
| ATOM | 450 | OE1 | GLU | 56 | 46.713 | 27.252 | 53.567 | 1.00 | 17.12 | AAAA |
| ATOM | 451 | OE2 | GLU | 56 | 47.773 | 26.564 | 55.394 | 1.00 | 18.23 | AAAA |
| ATOM | 452 | C | GLU | 56 | 43.781 | 23.313 | 52.000 | 1.00 | 15.95 | AAAA |
| ATOM | 453 | O | GLU | 56 | 42.799 | 22.869 | 52.599 | 1.00 | 17.82 | AAAA |
| ATOM | 454 | N | LEU | 57 | 43.722 | 23.691 | 50.725 | 1.00 | 17.53 | AAAA |
| ATOM | 455 | CA | LEU | 57 | 42.466 | 23.579 | 49.989 | 1.00 | 16.34 | AAAA |
| ATOM | 456 | CB | LEU | 57 | 42.591 | 24.177 | 48.586 | 1.00 | 13.86 | AAAA |
| ATOM | 457 | CG | LEU | 57 | 42.773 | 25.707 | 48.552 | 1.00 | 15.24 | AAAA |
| ATOM | 458 | CD1 | LEU | 57 | 42.923 | 26.182 | 47.101 | 1.00 | 19.30 | AAAA |
| ATOM | 459 | CD2 | LEU | 57 | 41.546 | 26.380 | 49.207 | 1.00 | 15.14 | AAAA |
| ATOM | 460 | C | LEU | 57 | 42.016 | 22.126 | 49.868 | 1.00 | 18.46 | AAAA |
| ATOM | 461 | O | LEU | 57 | 40.824 | 21.823 | 49.972 | 1.00 | 17.27 | AAAA |
| ATOM | 462 | N | LEU | 58 | 42.975 | 21.234 | 49.636 | 1.00 | 16.43 | AAAA |

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Figure 16-8

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 463 | CA | LEU | 58 | 42.662 | 19.822 | 49.475 | 1.00 | 15.18 | AAAA |
| ATOM | 464 | CB | LEU | 58 | 43.788 | 19.113 | 48.727 | 1.00 | 16.09 | AAAA |
| ATOM | 465 | CG | LEU | 58 | 44.029 | 19.682 | 47.321 | 1.00 | 21.72 | AAAA |
| ATOM | 466 | CD1 | LEU | 58 | 45.221 | 18.982 | 46.680 | 1.00 | 31.92 | AAAA |
| ATOM | 467 | CD2 | LEU | 58 | 42.786 | 19.549 | 46.469 | 1.00 | 34.38 | AAAA |
| ATOM | 468 | C | LEU | 58 | 42.339 | 19.116 | 50.787 | 1.00 | 21.19 | AAAA |
| ATOM | 469 | O | LEU | 58 | 42.067 | 17.914 | 50.795 | 1.00 | 20.40 | AAAA |
| ATOM | 470 | N | LEU | 59 | 42.377 | 19.849 | 51.896 | 1.00 | 13.50 | AAAA |
| ATOM | 471 | CA | LEU | 59 | 41.958 | 19.261 | 53.173 | 1.00 | 15.58 | AAAA |
| ATOM | 472 | CB | LEU | 59 | 42.182 | 20.236 | 54.339 | 1.00 | 18.98 | AAAA |
| ATOM | 473 | CG | LEU | 59 | 43.619 | 20.537 | 54.774 | 1.00 | 22.57 | AAAA |
| ATOM | 474 | CD1 | LEU | 59 | 43.640 | 21.654 | 55.808 | 1.00 | 19.88 | AAAA |
| ATOM | 475 | CD2 | LEU | 59 | 44.255 | 19.253 | 55.339 | 1.00 | 26.71 | AAAA |
| ATOM | 476 | C | LEU | 59 | 40.446 | 18.979 | 53.043 | 1.00 | 17.55 | AAAA |
| ATOM | 477 | O | LEU | 59 | 39.897 | 18.112 | 53.724 | 1.00 | 18.02 | AAAA |
| ATOM | 478 | N | PHE | 60 | 39.766 | 19.737 | 52.179 | 1.00 | 14.64 | AAAA |
| ATOM | 479 | CA | PHE | 60 | 38.338 | 19.536 | 51.970 | 1.00 | 18.17 | AAAA |
| ATOM | 480 | CB | PHE | 60 | 37.519 | 20.694 | 52.557 | 1.00 | 18.80 | AAAA |
| ATOM | 481 | CG | PHE | 60 | 36.028 | 20.564 | 52.316 | 1.00 | 15.94 | AAAA |
| ATOM | 482 | CD1 | PHE | 60 | 35.320 | 19.476 | 52.817 | 1.00 | 19.98 | AAAA |
| ATOM | 483 | CD2 | PHE | 60 | 35.339 | 21.524 | 51.576 | 1.00 | 18.09 | AAAA |
| ATOM | 484 | CE1 | PHE | 60 | 33.947 | 19.338 | 52.587 | 1.00 | 18.72 | AAAA |
| ATOM | 485 | CE2 | PHE | 60 | 33.964 | 21.399 | 51.338 | 1.00 | 19.19 | AAAA |
| ATOM | 486 | CZ | PHE | 60 | 33.268 | 20.295 | 51.850 | 1.00 | 18.43 | AAAA |
| ATOM | 487 | C | PHE | 60 | 37.916 | 19.337 | 50.510 | 1.00 | 16.45 | AAAA |
| ATOM | 488 | O | PHE | 60 | 37.227 | 18.371 | 50.179 | 1.00 | 19.18 | AAAA |
| ATOM | 489 | N | HIS | 61 | 38.308 | 20.257 | 49.638 | 1.00 | 18.26 | AAAA |
| ATOM | 490 | CA | HIS | 61 | 37.913 | 20.163 | 48.235 | 1.00 | 14.47 | AAAA |
| ATOM | 491 | CB | HIS | 61 | 38.004 | 21.545 | 47.582 | 1.00 | 17.15 | AAAA |
| ATOM | 492 | CG | HIS | 61 | 36.968 | 22.494 | 48.084 | 1.00 | 14.20 | AAAA |
| ATOM | 493 | CD2 | HIS | 61 | 35.645 | 22.580 | 47.816 | 1.00 | 11.05 | AAAA |
| ATOM | 494 | ND1 | HIS | 61 | 37.237 | 23.477 | 49.012 | 1.00 | 23.25 | AAAA |
| ATOM | 495 | CE1 | HIS | 61 | 36.121 | 24.131 | 49.291 | 1.00 | 13.35 | AAAA |
| ATOM | 496 | NE2 | HIS | 61 | 35.143 | 23.606 | 48.579 | 1.00 | 21.07 | AAAA |
| ATOM | 497 | C | HIS | 61 | 38.695 | 19.157 | 47.417 | 1.00 | 18.29 | AAAA |
| ATOM | 498 | O | HIS | 61 | 39.828 | 18.819 | 47.761 | 1.00 | 17.50 | AAAA |
| ATOM | 499 | N | THR | 62 | 38.071 | 18.658 | 46.346 | 1.00 | 15.39 | AAAA |
| ATOM | 500 | CA | THR | 62 | 38.741 | 17.686 | 45.473 | 1.00 | 19.02 | AAAA |
| ATOM | 501 | CB | THR | 62 | 37.734 | 16.767 | 44.756 | 1.00 | 19.61 | AAAA |
| ATOM | 502 | OG1 | THR | 62 | 36.795 | 17.548 | 44.006 | 1.00 | 22.05 | AAAA |
| ATOM | 503 | CG2 | THR | 62 | 36.995 | 15.925 | 45.767 | 1.00 | 28.99 | AAAA |
| ATOM | 504 | C | THR | 62 | 39.595 | 18.398 | 44.440 | 1.00 | 23.22 | AAAA |
| ATOM | 505 | O | THR | 62 | 39.311 | 19.532 | 44.044 | 1.00 | 17.47 | AAAA |
| ATOM | 506 | N | GLU | 63 | 40.657 | 17.732 | 44.009 | 1.00 | 18.94 | AAAA |
| ATOM | 507 | CA | GLU | 63 | 41.571 | 18.324 | 43.046 | 1.00 | 22.44 | AAAA |
| ATOM | 508 | CB | GLU | 63 | 42.736 | 17.384 | 42.750 | 1.00 | 28.31 | AAAA |
| ATOM | 509 | CG | GLU | 63 | 43.885 | 17.476 | 43.708 | 1.00 | 60.37 | AAAA |
| ATOM | 510 | CD | GLU | 63 | 45.154 | 16.893 | 43.115 | 1.00 | 65.08 | AAAA |
| ATOM | 511 | OE1 | GLU | 63 | 45.603 | 17.407 | 42.065 | 1.00 | 66.44 | AAAA |
| ATOM | 512 | OE2 | GLU | 63 | 45.697 | 15.927 | 43.694 | 1.00 | 71.72 | AAAA |
| ATOM | 513 | C | GLU | 63 | 40.983 | 18.764 | 41.730 | 1.00 | 18.63 | AAAA |
| ATOM | 514 | O | GLU | 63 | 41.340 | 19.827 | 41.228 | 1.00 | 18.37 | AAAA |
| ATOM | 515 | N | ASP | 64 | 40.108 | 17.943 | 41.153 | 1.00 | 19.77 | AAAA |
| ATOM | 516 | CA | ASP | 64 | 39.508 | 18.277 | 39.864 | 1.00 | 17.88 | AAAA |
| ATOM | 517 | CB | ASP | 64 | 38.584 | 17.159 | 39.372 | 1.00 | 20.43 | AAAA |
| ATOM | 518 | CG | ASP | 64 | 37.429 | 16.884 | 40.330 | 1.00 | 42.71 | AAAA |
| ATOM | 519 | OD1 | ASP | 64 | 36.415 | 16.291 | 39.899 | 1.00 | 45.01 | AAAA |
| ATOM | 520 | OD2 | ASP | 64 | 37.537 | 17.243 | 41.521 | 1.00 | 51.77 | AAAA |
| ATOM | 521 | C | ASP | 64 | 38.701 | 19.582 | 39.964 | 1.00 | 21.90 | AAAA |
| ATOM | 522 | O | ASP | 64 | 38.726 | 20.410 | 39.042 | 1.00 | 17.35 | AAAA |
| ATOM | 523 | N | TYR | 65 | 37.980 | 19.750 | 41.072 | 1.00 | 16.17 | AAAA |
| ATOM | 524 | CA | TYR | 65 | 37.178 | 20.957 | 41.292 | 1.00 | 15.62 | AAAA |
| ATOM | 525 | CB | TYR | 65 | 36.258 | 20.796 | 42.529 | 1.00 | 12.04 | AAAA |
| ATOM | 526 | CG | TYR | 65 | 35.501 | 22.065 | 42.886 | 1.00 | 12.23 | AAAA |
| ATOM | 527 | CD1 | TYR | 65 | 34.699 | 22.718 | 41.940 | 1.00 | 14.73 | AAAA |
| ATOM | 528 | CE1 | TYR | 65 | 34.028 | 23.910 | 42.253 | 1.00 | 18.23 | AAAA |

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Figure 16-9

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 529 | CD2 | TYR | 65 | 35.609 | 22.631 | 44.163 | 1.00 | 13.67 | AAAA |
| ATOM | 530 | CE2 | TYR | 65 | 34.943 | 23.824 | 44.486 | 1.00 | 18.16 | AAAA |
| ATOM | 531 | CZ | TYR | 65 | 34.162 | 24.461 | 43.533 | 1.00 | 16.88 | AAAA |
| ATOM | 532 | OH | TYR | 65 | 33.555 | 25.665 | 43.837 | 1.00 | 14.59 | AAAA |
| ATOM | 533 | C | TYR | 65 | 38.090 | 22.177 | 41.459 | 1.00 | 15.27 | AAAA |
| ATOM | 534 | O | TYR | 65 | 37.882 | 23.189 | 40.798 | 1.00 | 15.96 | AAAA |
| ATOM | 535 | N | ILE | 66 | 39.098 | 22.073 | 42.321 | 1.00 | 14.29 | AAAA |
| ATOM | 536 | CA | ILE | 66 | 40.022 | 23.179 | 42.540 | 1.00 | 18.86 | AAAA |
| ATOM | 537 | CB | ILE | 66 | 41.090 | 22.836 | 43.617 | 1.00 | 15.56 | AAAA |
| ATOM | 538 | CG2 | ILE | 66 | 42.152 | 23.943 | 43.698 | 1.00 | 20.45 | AAAA |
| ATOM | 539 | CG1 | ILE | 66 | 40.405 | 22.659 | 44.967 | 1.00 | 19.68 | AAAA |
| ATOM | 540 | CD1 | ILE | 66 | 39.717 | 23.948 | 45.454 | 1.00 | 29.11 | AAAA |
| ATOM | 541 | C | ILE | 66 | 40.716 | 23.519 | 41.236 | 1.00 | 25.20 | AAAA |
| ATOM | 542 | O | ILE | 66 | 40.809 | 24.692 | 40.895 | 1.00 | 14.60 | AAAA |
| ATOM | 543 | N | ASN | 67 | 41.190 | 22.508 | 40.498 | 1.00 | 18.21 | AAAA |
| ATOM | 544 | CA | ASN | 67 | 41.879 | 22.789 | 39.236 | 1.00 | 20.03 | AAAA |
| ATOM | 545 | CB | ASN | 67 | 42.448 | 21.523 | 38.580 | 1.00 | 21.73 | AAAA |
| ATOM | 546 | CG | ASN | 67 | 43.645 | 20.954 | 39.333 | 1.00 | 21.69 | AAAA |
| ATOM | 547 | OD1 | ASN | 67 | 44.293 | 21.645 | 40.110 | 1.00 | 23.97 | AAAA |
| ATOM | 548 | ND2 | ASN | 67 | 43.947 | 19.692 | 39.086 | 1.00 | 23.23 | AAAA |
| ATOM | 549 | C | ASN | 67 | 40.970 | 23.500 | 38.250 | 1.00 | 15.87 | AAAA |
| ATOM | 550 | O | ASN | 67 | 41.431 | 24.347 | 37.473 | 1.00 | 18.64 | AAAA |
| ATOM | 551 | N | THR | 68 | 39.681 | 23.180 | 38.295 | 1.00 | 16.55 | AAAA |
| ATOM | 552 | CA | THR | 68 | 38.729 | 23.814 | 37.400 | 1.00 | 20.34 | AAAA |
| ATOM | 553 | CB | THR | 68 | 37.360 | 23.114 | 37.441 | 1.00 | 22.99 | AAAA |
| ATOM | 554 | OG1 | THR | 68 | 37.511 | 21.760 | 36.978 | 1.00 | 21.75 | AAAA |
| ATOM | 555 | CG2 | THR | 68 | 36.378 | 23.827 | 36.536 | 1.00 | 17.37 | AAAA |
| ATOM | 556 | C | THR | 68 | 38.561 | 25.291 | 37.755 | 1.00 | 16.66 | AAAA |
| ATOM | 557 | O | THR | 68 | 38.472 | 26.139 | 36.871 | 1.00 | 18.79 | AAAA |
| ATOM | 558 | N | LEU | 69 | 38.534 | 25.604 | 39.045 | 1.00 | 14.82 | AAAA |
| ATOM | 559 | CA | LEU | 69 | 38.405 | 27.000 | 39.447 | 1.00 | 15.20 | AAAA |
| ATOM | 560 | CB | LEU | 69 | 38.295 | 27.126 | 40.973 | 1.00 | 16.87 | AAAA |
| ATOM | 561 | CG | LEU | 69 | 37.057 | 26.551 | 41.666 | 1.00 | 14.76 | AAAA |
| ATOM | 562 | CD1 | LEU | 69 | 37.212 | 26.643 | 43.179 | 1.00 | 16.81 | AAAA |
| ATOM | 563 | CD2 | LEU | 69 | 35.832 | 27.312 | 41.217 | 1.00 | 17.26 | AAAA |
| ATOM | 564 | C | LEU | 69 | 39.623 | 27.796 | 38.969 | 1.00 | 15.11 | AAAA |
| ATOM | 565 | O | LEU | 69 | 39.500 | 28.934 | 38.504 | 1.00 | 13.30 | AAAA |
| ATOM | 566 | N | MET | 70 | 40.803 | 27.204 | 39.090 | 1.00 | 13.40 | AAAA |
| ATOM | 567 | CA | MET | 70 | 42.019 | 27.894 | 38.659 | 1.00 | 16.97 | AAAA |
| ATOM | 568 | CB | MET | 70 | 43.254 | 27.114 | 39.075 | 1.00 | 14.87 | AAAA |
| ATOM | 569 | CG | MET | 70 | 43.335 | 26.886 | 40.582 | 1.00 | 15.18 | AAAA |
| ATOM | 570 | SD | MET | 70 | 44.828 | 25.954 | 41.060 | 1.00 | 28.71 | AAAA |
| ATOM | 571 | CE | MET | 70 | 46.051 | 27.228 | 40.893 | 1.00 | 21.19 | AAAA |
| ATOM | 572 | C | MET | 70 | 42.064 | 28.119 | 37.155 | 1.00 | 19.11 | AAAA |
| ATOM | 573 | O | MET | 70 | 42.498 | 29.170 | 36.700 | 1.00 | 17.10 | AAAA |
| ATOM | 574 | N | GLU | 71 | 41.648 | 27.118 | 36.389 | 1.00 | 15.06 | AAAA |
| ATOM | 575 | CA | GLU | 71 | 41.651 | 27.226 | 34.934 | 1.00 | 16.12 | AAAA |
| ATOM | 576 | CB | GLU | 71 | 41.397 | 25.856 | 34.305 | 1.00 | 16.12 | AAAA |
| ATOM | 577 | CG | GLU | 71 | 41.387 | 25.882 | 32.800 | 1.00 | 20.26 | AAAA |
| ATOM | 578 | CD | GLU | 71 | 42.782 | 25.920 | 32.193 | 1.00 | 32.31 | AAAA |
| ATOM | 579 | OE1 | GLU | 71 | 42.893 | 25.741 | 30.958 | 1.00 | 27.07 | AAAA |
| ATOM | 580 | OE2 | GLU | 71 | 43.762 | 26.117 | 32.941 | 1.00 | 24.85 | AAAA |
| ATOM | 581 | C | GLU | 71 | 40.580 | 28.208 | 34.466 | 1.00 | 16.48 | AAAA |
| ATOM | 582 | O | GLU | 71 | 40.831 | 29.066 | 33.611 | 1.00 | 17.20 | AAAA |
| ATOM | 583 | N | ALA | 72 | 39.380 | 28.097 | 35.027 | 1.00 | 15.68 | AAAA |
| ATOM | 584 | CA | ALA | 72 | 38.300 | 28.998 | 34.644 | 1.00 | 16.07 | AAAA |
| ATOM | 585 | CB | ALA | 72 | 37.035 | 28.669 | 35.425 | 1.00 | 17.21 | AAAA |
| ATOM | 586 | C | ALA | 72 | 38.678 | 30.453 | 34.897 | 1.00 | 19.07 | AAAA |
| ATOM | 587 | O | ALA | 72 | 38.448 | 31.326 | 34.054 | 1.00 | 15.92 | AAAA |
| ATOM | 588 | N | GLU | 73 | 39.260 | 30.726 | 36.062 | 1.00 | 15.86 | AAAA |
| ATOM | 589 | CA | GLU | 73 | 39.616 | 32.097 | 36.372 | 1.00 | 15.50 | AAAA |
| ATOM | 590 | CB | GLU | 73 | 40.046 | 32.210 | 37.828 | 1.00 | 14.12 | AAAA |
| ATOM | 591 | CG | GLU | 73 | 40.430 | 33.615 | 38.214 | 1.00 | 14.24 | AAAA |
| ATOM | 592 | CD | GLU | 73 | 40.961 | 33.699 | 39.629 | 1.00 | 17.23 | AAAA |
| ATOM | 593 | OE1 | GLU | 73 | 40.147 | 33.696 | 40.573 | 1.00 | 18.51 | AAAA |
| ATOM | 594 | OE2 | GLU | 73 | 42.201 | 33.753 | 39.793 | 1.00 | 20.88 | AAAA |

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Figure 16-10

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 595 | C | GLU | 73 | 40.706 | 32.709 | 35.495 | 1.00 | 20.36 | AAAA |
| ATOM | 596 | O | GLU | 73 | 40.527 | 33.806 | 34.948 | 1.00 | 17.74 | AAAA |
| ATOM | 597 | N | ARG | 74 | 41.832 | 32.020 | 35.344 | 1.00 | 21.57 | AAAA |
| ATOM | 598 | CA | ARG | 74 | 42.911 | 32.623 | 34.574 | 1.00 | 19.48 | AAAA |
| ATOM | 599 | CB | ARG | 74 | 44.256 | 31.912 | 34.834 | 1.00 | 18.48 | AAAA |
| ATOM | 600 | CG | ARG | 74 | 44.365 | 30.489 | 34.351 | 1.00 | 14.96 | AAAA |
| ATOM | 601 | CD | ARG | 74 | 45.723 | 29.892 | 34.745 | 1.00 | 15.05 | AAAA |
| ATOM | 602 | NE | ARG | 74 | 45.918 | 28.696 | 33.950 | 1.00 | 18.16 | AAAA |
| ATOM | 603 | CZ | ARG | 74 | 46.439 | 28.682 | 32.727 | 1.00 | 16.31 | AAAA |
| ATOM | 604 | NH1 | ARG | 74 | 46.843 | 29.811 | 32.145 | 1.00 | 19.74 | AAAA |
| ATOM | 605 | NH2 | ARG | 74 | 46.466 | 27.536 | 32.047 | 1.00 | 14.73 | AAAA |
| ATOM | 606 | C | ARG | 74 | 42.643 | 32.718 | 33.084 | 1.00 | 16.86 | AAAA |
| ATOM | 607 | O | ARG | 74 | 43.148 | 33.621 | 32.426 | 1.00 | 15.41 | AAAA |
| ATOM | 608 | N | CYS | 75 | 41.859 | 31.794 | 32.547 | 1.00 | 17.56 | AAAA |
| ATOM | 609 | CA | CYS | 75 | 41.544 | 31.833 | 31.115 | 1.00 | 18.24 | AAAA |
| ATOM | 610 | CB | CYS | 75 | 41.474 | 30.414 | 30.545 | 1.00 | 20.94 | AAAA |
| ATOM | 611 | SG | CYS | 75 | 43.047 | 29.514 | 30.572 | 1.00 | 19.30 | AAAA |
| ATOM | 612 | C | CYS | 75 | 40.216 | 32.561 | 30.898 | 1.00 | 15.81 | AAAA |
| ATOM | 613 | O | CYS | 75 | 39.762 | 32.748 | 29.762 | 1.00 | 17.79 | AAAA |
| ATOM | 614 | N | GLN | 76 | 39.601 | 32.959 | 32.007 | 1.00 | 15.63 | AAAA |
| ATOM | 615 | CA | GLN | 76 | 38.339 | 33.686 | 32.010 | 1.00 | 23.22 | AAAA |
| ATOM | 616 | CB | GLN | 76 | 38.595 | 35.122 | 31.530 | 1.00 | 22.99 | AAAA |
| ATOM | 617 | CG | GLN | 76 | 37.564 | 36.107 | 32.027 | 1.00 | 44.69 | AAAA |
| ATOM | 618 | CD | GLN | 76 | 37.588 | 36.229 | 33.535 | 1.00 | 47.78 | AAAA |
| ATOM | 619 | OE1 | GLN | 76 | 37.563 | 35.228 | 34.243 | 1.00 | 62.95 | AAAA |
| ATOM | 620 | NE2 | GLN | 76 | 37.619 | 37.452 | 34.033 | 1.00 | 45.96 | AAAA |
| ATOM | 621 | C | GLN | 76 | 37.304 | 32.975 | 31.135 | 1.00 | 23.43 | AAAA |
| ATOM | 622 | O | GLN | 76 | 36.826 | 33.512 | 30.135 | 1.00 | 19.93 | AAAA |
| ATOM | 623 | N | CYS | 77 | 36.951 | 31.754 | 31.521 | 1.00 | 15.97 | AAAA |
| ATOM | 624 | CA | CYS | 77 | 36.004 | 30.979 | 30.741 | 1.00 | 18.91 | AAAA |
| ATOM | 625 | CB | CYS | 77 | 36.738 | 30.225 | 29.623 | 1.00 | 24.64 | AAAA |
| ATOM | 626 | SG | CYS | 77 | 37.848 | 28.887 | 30.269 | 1.00 | 25.26 | AAAA |
| ATOM | 627 | C | CYS | 77 | 35.302 | 29.951 | 31.594 | 1.00 | 19.68 | AAAA |
| ATOM | 628 | O | CYS | 77 | 35.685 | 29.702 | 32.732 | 1.00 | 20.02 | AAAA |
| ATOM | 629 | N | VAL | 78 | 34.254 | 29.366 | 31.022 | 1.00 | 16.00 | AAAA |
| ATOM | 630 | CA | VAL | 78 | 33.531 | 28.288 | 31.671 | 1.00 | 18.73 | AAAA |
| ATOM | 631 | CB | VAL | 78 | 32.016 | 28.455 | 31.557 | 1.00 | 15.57 | AAAA |
| ATOM | 632 | CG1 | VAL | 78 | 31.312 | 27.304 | 32.262 | 1.00 | 21.27 | AAAA |
| ATOM | 633 | CG2 | VAL | 78 | 31.603 | 29.792 | 32.151 | 1.00 | 19.47 | AAAA |
| ATOM | 634 | C | VAL | 78 | 33.950 | 27.077 | 30.859 | 1.00 | 24.02 | AAAA |
| ATOM | 635 | O | VAL | 78 | 33.499 | 26.894 | 29.718 | 1.00 | 24.08 | AAAA |
| ATOM | 636 | N | PRO | 79 | 34.848 | 26.249 | 31.420 | 1.00 | 18.91 | AAAA |
| ATOM | 637 | CD | PRO | 79 | 35.470 | 26.341 | 32.756 | 1.00 | 17.70 | AAAA |
| ATOM | 638 | CA | PRO | 79 | 35.320 | 25.056 | 30.720 | 1.00 | 23.37 | AAAA |
| ATOM | 639 | CB | PRO | 79 | 36.295 | 24.432 | 31.732 | 1.00 | 21.92 | AAAA |
| ATOM | 640 | CG | PRO | 79 | 36.802 | 25.677 | 32.498 | 1.00 | 20.90 | AAAA |
| ATOM | 641 | C | PRO | 79 | 34.152 | 24.144 | 30.376 | 1.00 | 27.44 | AAAA |
| ATOM | 642 | O | PRO | 79 | 33.177 | 24.064 | 31.119 | 1.00 | 22.20 | AAAA |
| ATOM | 643 | N | LYS | 80 | 34.245 | 23.488 | 29.224 | 1.00 | 23.35 | AAAA |
| ATOM | 644 | CA | LYS | 80 | 33.212 | 22.570 | 28.775 | 1.00 | 26.78 | AAAA |
| ATOM | 645 | CB | LYS | 80 | 33.708 | 21.853 | 27.518 | 1.00 | 32.33 | AAAA |
| ATOM | 646 | CG | LYS | 80 | 35.098 | 21.256 | 27.680 | 1.00 | 51.34 | AAAA |
| ATOM | 647 | CD | LYS | 80 | 35.669 | 20.817 | 26.336 | 1.00 | 68.70 | AAAA |
| ATOM | 648 | CE | LYS | 80 | 37.131 | 20.401 | 26.451 | 1.00 | 70.04 | AAAA |
| ATOM | 649 | NZ | LYS | 80 | 37.688 | 19.949 | 25.141 | 1.00 | 73.72 | AAAA |
| ATOM | 650 | C | LYS | 80 | 32.875 | 21.571 | 29.875 | 1.00 | 24.71 | AAAA |
| ATOM | 651 | O | LYS | 80 | 33.770 | 20.957 | 30.458 | 1.00 | 24.23 | AAAA |
| ATOM | 652 | N | GLY | 81 | 31.582 | 21.431 | 30.161 | 1.00 | 16.74 | AAAA |
| ATOM | 653 | CA | GLY | 81 | 31.126 | 20.509 | 31.194 | 1.00 | 18.96 | AAAA |
| ATOM | 654 | C | GLY | 81 | 31.151 | 21.039 | 32.630 | 1.00 | 22.38 | AAAA |
| ATOM | 655 | O | GLY | 81 | 30.604 | 20.396 | 33.527 | 1.00 | 19.29 | AAAA |
| ATOM | 656 | N | ALA | 82 | 31.754 | 22.202 | 32.863 | 1.00 | 22.57 | AAAA |
| ATOM | 657 | CA | ALA | 82 | 31.858 | 22.738 | 34.235 | 1.00 | 20.65 | AAAA |
| ATOM | 658 | CB | ALA | 82 | 33.065 | 23.704 | 34.333 | 1.00 | 20.41 | AAAA |
| ATOM | 659 | C | ALA | 82 | 30.610 | 23.425 | 34.781 | 1.00 | 21.81 | AAAA |
| ATOM | 660 | O | ALA | 82 | 30.425 | 23.529 | 35.994 | 1.00 | 16.95 | AAAA |

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Figure 16-11

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 661 | N | ARG | 83 | 29.758 | 23.926 | 33.897 | 1.00 | 17.68 | AAAA |
| ATOM | 662 | CA | ARG | 83 | 28.549 | 24.596 | 34.360 | 1.00 | 15.04 | AAAA |
| ATOM | 663 | CB | ARG | 83 | 27.777 | 25.188 | 33.176 | 1.00 | 21.02 | AAAA |
| ATOM | 664 | CG | ARG | 83 | 26.938 | 26.395 | 33.528 | 1.00 | 36.77 | AAAA |
| ATOM | 665 | CD | ARG | 83 | 26.061 | 26.167 | 34.729 | 1.00 | 41.28 | AAAA |
| ATOM | 666 | NE | ARG | 83 | 25.366 | 27.393 | 35.105 | 1.00 | 40.05 | AAAA |
| ATOM | 667 | CZ | ARG | 83 | 24.530 | 27.492 | 36.134 | 1.00 | 51.15 | AAAA |
| ATOM | 668 | NH1 | ARG | 83 | 24.286 | 26.432 | 36.893 | 1.00 | 55.10 | AAAA |
| ATOM | 669 | NH2 | ARG | 83 | 23.931 | 28.646 | 36.399 | 1.00 | 54.26 | AAAA |
| ATOM | 670 | C | ARG | 83 | 27.701 | 23.530 | 35.030 | 1.00 | 21.33 | AAAA |
| ATOM | 671 | O | ARG | 83 | 27.193 | 23.708 | 36.130 | 1.00 | 24.88 | AAAA |
| ATOM | 672 | N | GLU | 84 | 27.565 | 22.406 | 34.352 | 1.00 | 18.76 | AAAA |
| ATOM | 673 | CA | GLU | 84 | 26.768 | 21.299 | 34.859 | 1.00 | 24.12 | AAAA |
| ATOM | 674 | CB | GLU | 84 | 26.527 | 20.290 | 33.744 | 1.00 | 32.64 | AAAA |
| ATOM | 675 | CG | GLU | 84 | 27.769 | 19.994 | 32.925 | 1.00 | 37.91 | AAAA |
| ATOM | 676 | CD | GLU | 84 | 27.832 | 20.784 | 31.612 | 1.00 | 51.24 | AAAA |
| ATOM | 677 | OE1 | GLU | 84 | 27.585 | 20.152 | 30.545 | 1.00 | 24.82 | AAAA |
| ATOM | 678 | OE2 | GLU | 84 | 28.114 | 22.018 | 31.650 | 1.00 | 22.57 | AAAA |
| ATOM | 679 | C | GLU | 84 | 27.394 | 20.570 | 36.043 | 1.00 | 25.36 | AAAA |
| ATOM | 680 | O | GLU | 84 | 26.739 | 20.321 | 37.057 | 1.00 | 26.17 | AAAA |
| ATOM | 681 | N | LYS | 85 | 28.665 | 20.232 | 35.897 | 1.00 | 18.78 | AAAA |
| ATOM | 682 | CA | LYS | 85 | 29.399 | 19.497 | 36.915 | 1.00 | 20.03 | AAAA |
| ATOM | 683 | CB | LYS | 85 | 30.658 | 18.900 | 36.280 | 1.00 | 18.59 | AAAA |
| ATOM | 684 | CG | LYS | 85 | 31.603 | 18.223 | 37.268 | 1.00 | 35.69 | AAAA |
| ATOM | 685 | CD | LYS | 85 | 31.151 | 16.832 | 37.644 | 1.00 | 51.51 | AAAA |
| ATOM | 686 | CE | LYS | 85 | 31.451 | 15.864 | 36.520 | 1.00 | 59.18 | AAAA |
| ATOM | 687 | NZ | LYS | 85 | 32.914 | 15.858 | 36.240 | 1.00 | 56.63 | AAAA |
| ATOM | 688 | C | LYS | 85 | 29.611 | 20.263 | 38.181 | 1.00 | 18.31 | AAAA |
| ATOM | 689 | O | LYS | 85 | 29.696 | 19.738 | 39.290 | 1.00 | 21.65 | AAAA |
| ATOM | 690 | N | TYR | 86 | 30.274 | 21.495 | 38.012 | 1.00 | 19.45 | AAAA |
| ATOM | 691 | CA | TYR | 86 | 30.776 | 22.272 | 39.145 | 1.00 | 14.26 | AAAA |
| ATOM | 692 | CB | TYR | 86 | 32.207 | 22.692 | 38.840 | 1.00 | 14.95 | AAAA |
| ATOM | 693 | CG | TYR | 86 | 33.107 | 21.508 | 38.585 | 1.00 | 19.76 | AAAA |
| ATOM | 694 | CD1 | TYR | 86 | 33.384 | 20.591 | 39.601 | 1.00 | 18.83 | AAAA |
| ATOM | 695 | CE1 | TYR | 86 | 34.247 | 19.519 | 39.388 | 1.00 | 20.29 | AAAA |
| ATOM | 696 | CD2 | TYR | 86 | 33.711 | 21.322 | 37.337 | 1.00 | 18.14 | AAAA |
| ATOM | 697 | CE2 | TYR | 86 | 34.567 | 20.261 | 37.112 | 1.00 | 22.66 | AAAA |
| ATOM | 698 | CZ | TYR | 86 | 34.832 | 19.364 | 38.145 | 1.00 | 22.61 | AAAA |
| ATOM | 699 | OH | TYR | 86 | 35.680 | 18.317 | 37.921 | 1.00 | 23.68 | AAAA |
| ATOM | 700 | C | TYR | 86 | 29.967 | 23.493 | 39.526 | 1.00 | 19.03 | AAAA |
| ATOM | 701 | O | TYR | 86 | 30.353 | 24.226 | 40.450 | 1.00 | 19.18 | AAAA |
| ATOM | 702 | N | ASN | 87 | 28.873 | 23.721 | 38.803 | 1.00 | 17.59 | AAAA |
| ATOM | 703 | CA | ASN | 87 | 27.953 | 24.843 | 39.071 | 1.00 | 18.07 | AAAA |
| ATOM | 704 | CB | ASN | 87 | 27.413 | 24.730 | 40.514 | 1.00 | 23.87 | AAAA |
| ATOM | 705 | CG | ASN | 87 | 26.020 | 25.349 | 40.688 | 1.00 | 30.67 | AAAA |
| ATOM | 706 | OD1 | ASN | 87 | 25.531 | 25.520 | 41.819 | 1.00 | 31.55 | AAAA |
| ATOM | 707 | ND2 | ASN | 87 | 25.370 | 25.661 | 39.580 | 1.00 | 20.18 | AAAA |
| ATOM | 708 | C | ASN | 87 | 28.641 | 26.197 | 38.875 | 1.00 | 24.24 | AAAA |
| ATOM | 709 | O | ASN | 87 | 28.283 | 27.190 | 39.519 | 1.00 | 18.57 | AAAA |
| ATOM | 710 | N | ILE | 88 | 29.617 | 26.237 | 37.970 | 1.00 | 18.80 | AAAA |
| ATOM | 711 | CA | ILE | 88 | 30.353 | 27.471 | 37.680 | 1.00 | 18.55 | AAAA |
| ATOM | 712 | CB | ILE | 88 | 31.865 | 27.166 | 37.508 | 1.00 | 26.44 | AAAA |
| ATOM | 713 | CG2 | ILE | 88 | 32.613 | 28.406 | 37.044 | 1.00 | 43.71 | AAAA |
| ATOM | 714 | CG1 | ILE | 88 | 32.439 | 26.703 | 38.835 | 1.00 | 36.30 | AAAA |
| ATOM | 715 | CD1 | ILE | 88 | 32.295 | 27.735 | 39.888 | 1.00 | 24.08 | AAAA |
| ATOM | 716 | C | ILE | 88 | 29.887 | 28.142 | 36.392 | 1.00 | 14.36 | AAAA |
| ATOM | 717 | O | ILE | 88 | 29.584 | 27.459 | 35.426 | 1.00 | 21.93 | AAAA |
| ATOM | 718 | N | GLY | 89 | 29.843 | 29.473 | 36.380 | 1.00 | 18.71 | AAAA |
| ATOM | 719 | CA | GLY | 89 | 29.479 | 30.162 | 35.154 | 1.00 | 20.23 | AAAA |
| ATOM | 720 | C | GLY | 89 | 28.147 | 30.873 | 35.106 | 1.00 | 20.85 | AAAA |
| ATOM | 721 | O | GLY | 89 | 28.006 | 31.817 | 34.330 | 1.00 | 25.47 | AAAA |
| ATOM | 722 | N | GLY | 90 | 27.172 | 30.414 | 35.889 | 1.00 | 21.17 | AAAA |
| ATOM | 723 | CA | GLY | 90 | 25.863 | 31.060 | 35.898 | 1.00 | 24.44 | AAAA |
| ATOM | 724 | C | GLY | 90 | 25.862 | 32.371 | 36.668 | 1.00 | 30.60 | AAAA |
| ATOM | 725 | O | GLY | 90 | 26.900 | 32.788 | 37.168 | 1.00 | 28.13 | AAAA |
| ATOM | 726 | N | TYR | 91 | 24.708 | 33.036 | 36.755 | 1.00 | 23.38 | AAAA |

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Figure 16-12

| | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 727 | CA | TYR | 91 | 24.598 | 34.299 | 37.490 | 1.00 | 28.48 | AAAA |
| ATOM | 728 | CB | TYR | 91 | 23.144 | 34.753 | 37.545 | 1.00 | 29.88 | AAAA |
| ATOM | 729 | CG | TYR | 91 | 22.923 | 35.899 | 38.518 | 1.00 | 33.88 | AAAA |
| ATOM | 730 | CD1 | TYR | 91 | 23.329 | 37.197 | 38.207 | 1.00 | 39.69 | AAAA |
| ATOM | 731 | CE1 | TYR | 91 | 23.130 | 38.250 | 39.104 | 1.00 | 31.76 | AAAA |
| ATOM | 732 | CD2 | TYR | 91 | 22.317 | 35.678 | 39.759 | 1.00 | 40.63 | AAAA |
| ATOM | 733 | CE2 | TYR | 91 | 22.115 | 36.720 | 40.664 | 1.00 | 37.07 | AAAA |
| ATOM | 734 | CZ | TYR | 91 | 22.521 | 38.002 | 40.327 | 1.00 | 36.22 | AAAA |
| ATOM | 735 | OH | TYR | 91 | 22.306 | 39.035 | 41.210 | 1.00 | 44.71 | AAAA |
| ATOM | 736 | C | TYR | 91 | 25.075 | 34.157 | 38.937 | 1.00 | 23.59 | AAAA |
| ATOM | 737 | O | TYR | 91 | 25.713 | 35.041 | 39.502 | 1.00 | 22.84 | AAAA |
| ATOM | 738 | N | GLU | 92 | 24.724 | 33.032 | 39.531 | 1.00 | 23.09 | AAAA |
| ATOM | 739 | CA | GLU | 92 | 25.048 | 32.747 | 40.917 | 1.00 | 26.61 | AAAA |
| ATOM | 740 | CB | GLU | 92 | 24.289 | 31.476 | 41.306 | 1.00 | 32.57 | AAAA |
| ATOM | 741 | CG | GLU | 92 | 24.595 | 30.892 | 42.657 | 1.00 | 41.38 | AAAA |
| ATOM | 742 | CD | GLU | 92 | 23.604 | 29.800 | 43.023 | 1.00 | 49.02 | AAAA |
| ATOM | 743 | OE1 | GLU | 92 | 24.008 | 28.829 | 43.715 | 1.00 | 45.51 | AAAA |
| ATOM | 744 | OE2 | GLU | 92 | 22.418 | 29.931 | 42.628 | 1.00 | 38.16 | AAAA |
| ATOM | 745 | C | GLU | 92 | 26.541 | 32.636 | 41.251 | 1.00 | 25.78 | AAAA |
| ATOM | 746 | O | GLU | 92 | 27.045 | 33.358 | 42.125 | 1.00 | 24.95 | AAAA |
| ATOM | 747 | N | ASN | 93 | 27.243 | 31.742 | 40.556 | 1.00 | 21.41 | AAAA |
| ATOM | 748 | CA | ASN | 93 | 28.674 | 31.519 | 40.777 | 1.00 | 21.14 | AAAA |
| ATOM | 749 | CB | ASN | 93 | 28.876 | 30.075 | 41.226 | 1.00 | 17.27 | AAAA |
| ATOM | 750 | CG | ASN | 93 | 27.905 | 29.682 | 42.320 | 1.00 | 15.34 | AAAA |
| ATOM | 751 | OD1 | ASN | 93 | 27.882 | 30.290 | 43.399 | 1.00 | 20.33 | AAAA |
| ATOM | 752 | ND2 | ASN | 93 | 27.078 | 28.674 | 42.047 | 1.00 | 20.49 | AAAA |
| ATOM | 753 | C | ASN | 93 | 29.378 | 31.778 | 39.445 | 1.00 | 22.25 | AAAA |
| ATOM | 754 | O | ASN | 93 | 29.901 | 30.865 | 38.806 | 1.00 | 20.29 | AAAA |
| ATOM | 755 | N | PRO | 94 | 29.451 | 33.057 | 39.045 | 1.00 | 25.45 | AAAA |
| ATOM | 756 | CD | PRO | 94 | 29.027 | 34.221 | 39.839 | 1.00 | 23.03 | AAAA |
| ATOM | 757 | CA | PRO | 94 | 30.055 | 33.523 | 37.794 | 1.00 | 23.05 | AAAA |
| ATOM | 758 | CB | PRO | 94 | 29.669 | 35.004 | 37.759 | 1.00 | 28.71 | AAAA |
| ATOM | 759 | CG | PRO | 94 | 28.528 | 35.112 | 38.755 | 1.00 | 40.02 | AAAA |
| ATOM | 760 | C | PRO | 94 | 31.554 | 33.384 | 37.697 | 1.00 | 26.51 | AAAA |
| ATOM | 761 | O | PRO | 94 | 32.232 | 33.185 | 38.688 | 1.00 | 17.36 | AAAA |
| ATOM | 762 | N | VAL | 95 | 32.068 | 33.498 | 36.478 | 1.00 | 21.12 | AAAA |
| ATOM | 763 | CA | VAL | 95 | 33.506 | 33.493 | 36.281 | 1.00 | 17.00 | AAAA |
| ATOM | 764 | CB | VAL | 95 | 33.851 | 33.242 | 34.796 | 1.00 | 25.15 | AAAA |
| ATOM | 765 | CG1 | VAL | 95 | 35.326 | 33.537 | 34.533 | 1.00 | 27.19 | AAAA |
| ATOM | 766 | CG2 | VAL | 95 | 33.551 | 31.791 | 34.443 | 1.00 | 17.37 | AAAA |
| ATOM | 767 | C | VAL | 95 | 33.989 | 34.899 | 36.686 | 1.00 | 17.42 | AAAA |
| ATOM | 768 | O | VAL | 95 | 33.426 | 35.894 | 36.237 | 1.00 | 23.43 | AAAA |
| ATOM | 769 | N | SER | 96 | 34.986 | 34.982 | 37.563 | 1.00 | 18.84 | AAAA |
| ATOM | 770 | CA | SER | 96 | 35.564 | 36.270 | 37.982 | 1.00 | 21.77 | AAAA |
| ATOM | 771 | CB | SER | 96 | 34.608 | 37.070 | 38.867 | 1.00 | 23.11 | AAAA |
| ATOM | 772 | OG | SER | 96 | 34.723 | 36.679 | 40.223 | 1.00 | 24.43 | AAAA |
| ATOM | 773 | C | SER | 96 | 36.835 | 35.987 | 38.789 | 1.00 | 29.09 | AAAA |
| ATOM | 774 | O | SER | 96 | 37.117 | 34.828 | 39.115 | 1.00 | 27.12 | AAAA |
| ATOM | 775 | N | TYR | 97 | 37.610 | 37.020 | 39.124 | 1.00 | 17.51 | AAAA |
| ATOM | 776 | CA | TYR | 97 | 38.803 | 36.751 | 39.911 | 1.00 | 20.69 | AAAA |
| ATOM | 777 | CB | TYR | 97 | 39.865 | 37.835 | 39.712 | 1.00 | 21.82 | AAAA |
| ATOM | 778 | CG | TYR | 97 | 40.492 | 37.748 | 38.332 | 1.00 | 22.72 | AAAA |
| ATOM | 779 | CD1 | TYR | 97 | 39.936 | 38.414 | 37.235 | 1.00 | 28.47 | AAAA |
| ATOM | 780 | CE1 | TYR | 97 | 40.473 | 38.265 | 35.949 | 1.00 | 24.45 | AAAA |
| ATOM | 781 | CD2 | TYR | 97 | 41.599 | 36.929 | 38.112 | 1.00 | 19.74 | AAAA |
| ATOM | 782 | CE2 | TYR | 97 | 42.144 | 36.771 | 36.832 | 1.00 | 21.63 | AAAA |
| ATOM | 783 | CZ | TYR | 97 | 41.578 | 37.439 | 35.759 | 1.00 | 23.13 | AAAA |
| ATOM | 784 | OH | TYR | 97 | 42.122 | 37.273 | 34.501 | 1.00 | 28.54 | AAAA |
| ATOM | 785 | C | TYR | 97 | 38.510 | 36.515 | 41.393 | 1.00 | 20.12 | AAAA |
| ATOM | 786 | O | TYR | 97 | 39.413 | 36.285 | 42.194 | 1.00 | 19.76 | AAAA |
| ATOM | 787 | N | ALA | 98 | 37.243 | 36.558 | 41.764 | 1.00 | 18.56 | AAAA |
| ATOM | 788 | CA | ALA | 98 | 36.899 | 36.259 | 43.139 | 1.00 | 22.23 | AAAA |
| ATOM | 789 | CB | ALA | 98 | 35.561 | 36.888 | 43.515 | 1.00 | 27.92 | AAAA |
| ATOM | 790 | C | ALA | 98 | 36.776 | 34.743 | 43.224 | 1.00 | 23.56 | AAAA |
| ATOM | 791 | O | ALA | 98 | 36.931 | 34.166 | 44.289 | 1.00 | 20.14 | AAAA |
| ATOM | 792 | N | MET | 99 | 36.538 | 34.094 | 42.087 | 1.00 | 16.84 | AAAA |

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Figure 16-13

| | | | | | | | | | | |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 793 | CA | MET | 99 | 36.295 | 32.643 | 42.117 | 1.00 | 17.60 | AAAA |
| ATOM | 794 | CB | MET | 99 | 35.864 | 32.137 | 40.736 | 1.00 | 17.05 | AAAA |
| ATOM | 795 | CG | MET | 99 | 36.999 | 31.824 | 39.793 | 1.00 | 11.16 | AAAA |
| ATOM | 796 | SD | MET | 99 | 36.314 | 31.698 | 38.113 | 1.00 | 16.54 | AAAA |
| ATOM | 797 | CE | MET | 99 | 35.165 | 30.295 | 38.312 | 1.00 | 17.83 | AAAA |
| ATOM | 798 | C | MET | 99 | 37.432 | 31.800 | 42.650 | 1.00 | 18.98 | AAAA |
| ATOM | 799 | O | MET | 99 | 37.197 | 30.753 | 43.251 | 1.00 | 18.21 | AAAA |
| ATOM | 800 | N | PHE | 100 | 38.670 | 32.216 | 42.420 | 1.00 | 12.87 | AAAA |
| ATOM | 801 | CA | PHE | 100 | 39.774 | 31.439 | 42.987 | 1.00 | 17.13 | AAAA |
| ATOM | 802 | CB | PHE | 100 | 40.559 | 30.681 | 41.917 | 1.00 | 15.23 | AAAA |
| ATOM | 803 | CG | PHE | 100 | 41.647 | 29.834 | 42.492 | 1.00 | 15.20 | AAAA |
| ATOM | 804 | CD1 | PHE | 100 | 41.342 | 28.638 | 43.140 | 1.00 | 22.96 | AAAA |
| ATOM | 805 | CD2 | PHE | 100 | 42.972 | 30.282 | 42.488 | 1.00 | 17.12 | AAAA |
| ATOM | 806 | CE1 | PHE | 100 | 42.341 | 27.901 | 43.782 | 1.00 | 19.23 | AAAA |
| ATOM | 807 | CE2 | PHE | 100 | 43.974 | 29.552 | 43.129 | 1.00 | 16.99 | AAAA |
| ATOM | 808 | CZ | PHE | 100 | 43.658 | 28.360 | 43.779 | 1.00 | 17.78 | AAAA |
| ATOM | 809 | C | PHE | 100 | 40.755 | 32.305 | 43.774 | 1.00 | 20.54 | AAAA |
| ATOM | 810 | O | PHE | 100 | 41.088 | 31.990 | 44.912 | 1.00 | 21.45 | AAAA |
| ATOM | 811 | N | THR | 101 | 41.219 | 33.401 | 43.187 | 1.00 | 18.02 | AAAA |
| ATOM | 812 | CA | THR | 101 | 42.177 | 34.245 | 43.902 | 1.00 | 15.25 | AAAA |
| ATOM | 813 | CB | THR | 101 | 42.715 | 35.341 | 42.976 | 1.00 | 16.33 | AAAA |
| ATOM | 814 | OG1 | THR | 101 | 43.386 | 34.720 | 41.870 | 1.00 | 16.01 | AAAA |
| ATOM | 815 | CG2 | THR | 101 | 43.706 | 36.226 | 43.697 | 1.00 | 16.31 | AAAA |
| ATOM | 816 | C | THR | 101 | 41.567 | 34.860 | 45.160 | 1.00 | 14.12 | AAAA |
| ATOM | 817 | O | THR | 101 | 42.110 | 34.707 | 46.244 | 1.00 | 16.86 | AAAA |
| ATOM | 818 | N | GLY | 102 | 40.435 | 35.541 | 45.008 | 1.00 | 13.77 | AAAA |
| ATOM | 819 | CA | GLY | 102 | 39.770 | 36.145 | 46.156 | 1.00 | 16.29 | AAAA |
| ATOM | 820 | C | GLY | 102 | 39.330 | 35.065 | 47.133 | 1.00 | 16.75 | AAAA |
| ATOM | 821 | O | GLY | 102 | 39.502 | 35.202 | 48.338 | 1.00 | 14.48 | AAAA |
| ATOM | 822 | N | SER | 103 | 38.752 | 33.986 | 46.615 | 1.00 | 16.24 | AAAA |
| ATOM | 823 | CA | SER | 103 | 38.315 | 32.890 | 47.488 | 1.00 | 16.72 | AAAA |
| ATOM | 824 | CB | SER | 103 | 37.567 | 31.821 | 46.684 | 1.00 | 15.97 | AAAA |
| ATOM | 825 | OG | SER | 103 | 36.339 | 32.349 | 46.197 | 1.00 | 26.86 | AAAA |
| ATOM | 826 | C | SER | 103 | 39.494 | 32.264 | 48.218 | 1.00 | 17.88 | AAAA |
| ATOM | 827 | O | SER | 103 | 39.405 | 31.974 | 49.419 | 1.00 | 14.17 | AAAA |
| ATOM | 828 | N | SER | 104 | 40.604 | 32.057 | 47.515 | 1.00 | 11.40 | AAAA |
| ATOM | 829 | CA | SER | 104 | 41.780 | 31.484 | 48.181 | 1.00 | 17.61 | AAAA |
| ATOM | 830 | CB | SER | 104 | 42.888 | 31.206 | 47.160 | 1.00 | 15.89 | AAAA |
| ATOM | 831 | OG | SER | 104 | 42.525 | 30.102 | 46.362 | 1.00 | 27.82 | AAAA |
| ATOM | 832 | C | SER | 104 | 42.332 | 32.404 | 49.271 | 1.00 | 17.02 | AAAA |
| ATOM | 833 | O | SER | 104 | 42.867 | 31.958 | 50.286 | 1.00 | 15.37 | AAAA |
| ATOM | 834 | N | LEU | 105 | 42.206 | 33.698 | 49.052 | 1.00 | 17.10 | AAAA |
| ATOM | 835 | CA | LEU | 105 | 42.709 | 34.652 | 50.016 | 1.00 | 16.95 | AAAA |
| ATOM | 836 | CB | LEU | 105 | 42.728 | 36.037 | 49.365 | 1.00 | 18.44 | AAAA |
| ATOM | 837 | CG | LEU | 105 | 43.613 | 37.108 | 49.981 | 1.00 | 29.88 | AAAA |
| ATOM | 838 | CD1 | LEU | 105 | 45.086 | 36.631 | 49.959 | 1.00 | 20.25 | AAAA |
| ATOM | 839 | CD2 | LEU | 105 | 43.438 | 38.418 | 49.175 | 1.00 | 29.39 | AAAA |
| ATOM | 840 | C | LEU | 105 | 41.837 | 34.637 | 51.282 | 1.00 | 14.81 | AAAA |
| ATOM | 841 | O | LEU | 105 | 42.334 | 34.703 | 52.404 | 1.00 | 17.74 | AAAA |
| ATOM | 842 | N | ALA | 106 | 40.532 | 34.531 | 51.095 | 1.00 | 19.28 | AAAA |
| ATOM | 843 | CA | ALA | 106 | 39.601 | 34.493 | 52.224 | 1.00 | 12.39 | AAAA |
| ATOM | 844 | CB | ALA | 106 | 38.140 | 34.574 | 51.704 | 1.00 | 11.58 | AAAA |
| ATOM | 845 | C | ALA | 106 | 39.807 | 33.210 | 53.023 | 1.00 | 14.79 | AAAA |
| ATOM | 846 | O | ALA | 106 | 39.704 | 33.203 | 54.250 | 1.00 | 13.58 | AAAA |
| ATOM | 847 | N | THR | 107 | 40.114 | 32.128 | 52.318 | 1.00 | 13.67 | AAAA |
| ATOM | 848 | CA | THR | 107 | 40.314 | 30.819 | 52.956 | 1.00 | 13.21 | AAAA |
| ATOM | 849 | CB | THR | 107 | 40.187 | 29.708 | 51.902 | 1.00 | 14.95 | AAAA |
| ATOM | 850 | OG1 | THR | 107 | 38.868 | 29.792 | 51.334 | 1.00 | 15.72 | AAAA |
| ATOM | 851 | CG2 | THR | 107 | 40.422 | 28.311 | 52.511 | 1.00 | 9.51 | AAAA |
| ATOM | 852 | C | THR | 107 | 41.649 | 30.751 | 53.687 | 1.00 | 15.80 | AAAA |
| ATOM | 853 | O | THR | 107 | 41.734 | 30.206 | 54.792 | 1.00 | 15.63 | AAAA |
| ATOM | 854 | N | GLY | 108 | 42.696 | 31.294 | 53.082 | 1.00 | 14.08 | AAAA |
| ATOM | 855 | CA | GLY | 108 | 43.968 | 31.298 | 53.765 | 1.00 | 14.62 | AAAA |
| ATOM | 856 | C | GLY | 108 | 43.801 | 32.119 | 55.041 | 1.00 | 20.05 | AAAA |
| ATOM | 857 | O | GLY | 108 | 44.417 | 31.813 | 56.063 | 1.00 | 17.53 | AAAA |
| ATOM | 858 | N | SER | 109 | 42.963 | 33.158 | 54.988 | 1.00 | 15.26 | AAAA |

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Figure 16-14

| | | | | | | | | | | |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 859 | CA | SER | 109 | 42.727 | 34.020 | 56.153 | 1.00 | 14.54 | AAAA |
| ATOM | 860 | CB | SER | 109 | 41.906 | 35.248 | 55.737 | 1.00 | 15.58 | AAAA |
| ATOM | 861 | OG | SER | 109 | 42.627 | 36.045 | 54.809 | 1.00 | 16.97 | AAAA |
| ATOM | 862 | C | SER | 109 | 42.037 | 33.264 | 57.297 | 1.00 | 15.56 | AAAA |
| ATOM | 863 | O | SER | 109 | 42.189 | 33.600 | 58.487 | 1.00 | 17.00 | AAAA |
| ATOM | 864 | N | THR | 110 | 41.261 | 32.247 | 56.944 | 1.00 | 14.37 | AAAA |
| ATOM | 865 | CA | THR | 110 | 40.608 | 31.435 | 57.957 | 1.00 | 12.89 | AAAA |
| ATOM | 866 | CB | THR | 110 | 39.452 | 30.628 | 57.360 | 1.00 | 14.54 | AAAA |
| ATOM | 867 | OG1 | THR | 110 | 38.346 | 31.519 | 57.163 | 1.00 | 18.11 | AAAA |
| ATOM | 868 | CG2 | THR | 110 | 39.061 | 29.452 | 58.278 | 1.00 | 12.91 | AAAA |
| ATOM | 869 | C | THR | 110 | 41.633 | 30.524 | 58.601 | 1.00 | 18.44 | AAAA |
| ATOM | 870 | O | THR | 110 | 41.574 | 30.302 | 59.806 | 1.00 | 16.30 | AAAA |
| ATOM | 871 | N | VAL | 111 | 42.584 | 30.013 | 57.816 | 1.00 | 15.20 | AAAA |
| ATOM | 872 | CA | VAL | 111 | 43.614 | 29.180 | 58.403 | 1.00 | 20.45 | AAAA |
| ATOM | 873 | CB | VAL | 111 | 44.517 | 28.514 | 57.323 | 1.00 | 20.02 | AAAA |
| ATOM | 874 | CG1 | VAL | 111 | 45.652 | 27.765 | 58.005 | 1.00 | 21.79 | AAAA |
| ATOM | 875 | CG2 | VAL | 111 | 43.697 | 27.537 | 56.482 | 1.00 | 19.07 | AAAA |
| ATOM | 876 | C | VAL | 111 | 44.456 | 30.075 | 59.327 | 1.00 | 18.21 | AAAA |
| ATOM | 877 | O | VAL | 111 | 44.838 | 29.672 | 60.431 | 1.00 | 18.65 | AAAA |
| ATOM | 878 | N | GLN | 112 | 44.731 | 31.302 | 58.890 | 1.00 | 16.82 | AAAA |
| ATOM | 879 | CA | GLN | 112 | 45.493 | 32.232 | 59.719 | 1.00 | 20.13 | AAAA |
| ATOM | 880 | CB | GLN | 112 | 45.751 | 33.540 | 58.970 | 1.00 | 22.39 | AAAA |
| ATOM | 881 | CG | GLN | 112 | 46.593 | 33.360 | 57.723 | 1.00 | 21.17 | AAAA |
| ATOM | 882 | CD | GLN | 112 | 46.797 | 34.651 | 56.982 | 1.00 | 24.82 | AAAA |
| ATOM | 883 | OE1 | GLN | 112 | 47.772 | 35.381 | 57.219 | 1.00 | 25.62 | AAAA |
| ATOM | 884 | NE2 | GLN | 112 | 45.866 | 34.963 | 56.091 | 1.00 | 13.16 | AAAA |
| ATOM | 885 | C | GLN | 112 | 44.743 | 32.516 | 61.012 | 1.00 | 23.99 | AAAA |
| ATOM | 886 | O | GLN | 112 | 45.340 | 32.593 | 62.079 | 1.00 | 17.94 | AAAA |
| ATOM | 887 | N | ALA | 113 | 43.431 | 32.700 | 60.924 | 1.00 | 15.60 | AAAA |
| ATOM | 888 | CA | ALA | 113 | 42.653 | 32.941 | 62.138 | 1.00 | 15.04 | AAAA |
| ATOM | 889 | CB | ALA | 113 | 41.191 | 33.138 | 61.802 | 1.00 | 18.65 | AAAA |
| ATOM | 890 | C | ALA | 113 | 42.807 | 31.751 | 63.083 | 1.00 | 14.84 | AAAA |
| ATOM | 891 | O | ALA | 113 | 42.941 | 31.909 | 64.296 | 1.00 | 21.05 | AAAA |
| ATOM | 892 | N | ILE | 114 | 42.767 | 30.550 | 62.534 | 1.00 | 16.45 | AAAA |
| ATOM | 893 | CA | ILE | 114 | 42.919 | 29.383 | 63.389 | 1.00 | 15.38 | AAAA |
| ATOM | 894 | CB | ILE | 114 | 42.600 | 28.100 | 62.637 | 1.00 | 15.22 | AAAA |
| ATOM | 895 | CG2 | ILE | 114 | 42.888 | 26.893 | 63.537 | 1.00 | 15.72 | AAAA |
| ATOM | 896 | CG1 | ILE | 114 | 41.110 | 28.112 | 62.244 | 1.00 | 19.28 | AAAA |
| ATOM | 897 | CD1 | ILE | 114 | 40.744 | 27.038 | 61.191 | 1.00 | 13.43 | AAAA |
| ATOM | 898 | C | ILE | 114 | 44.329 | 29.318 | 63.968 | 1.00 | 18.02 | AAAA |
| ATOM | 899 | O | ILE | 114 | 44.508 | 28.998 | 65.156 | 1.00 | 20.38 | AAAA |
| ATOM | 900 | N | GLU | 115 | 45.328 | 29.629 | 63.144 | 1.00 | 15.27 | AAAA |
| ATOM | 901 | CA | GLU | 115 | 46.726 | 29.626 | 63.614 | 1.00 | 21.48 | AAAA |
| ATOM | 902 | CB | GLU | 115 | 47.690 | 30.080 | 62.506 | 1.00 | 21.76 | AAAA |
| ATOM | 903 | CG | GLU | 115 | 47.884 | 29.080 | 61.386 | 1.00 | 15.78 | AAAA |
| ATOM | 904 | CD | GLU | 115 | 48.670 | 29.648 | 60.211 | 1.00 | 20.04 | AAAA |
| ATOM | 905 | OE1 | GLU | 115 | 49.051 | 30.843 | 60.239 | 1.00 | 21.48 | AAAA |
| ATOM | 906 | OE2 | GLU | 115 | 48.901 | 28.902 | 59.241 | 1.00 | 26.59 | AAAA |
| ATOM | 907 | C | GLU | 115 | 46.877 | 30.559 | 64.814 | 1.00 | 23.55 | AAAA |
| ATOM | 908 | O | GLU | 115 | 47.509 | 30.212 | 65.815 | 1.00 | 23.03 | AAAA |
| ATOM | 909 | N | GLU | 116 | 46.295 | 31.748 | 64.703 | 1.00 | 22.73 | AAAA |
| ATOM | 910 | CA | GLU | 116 | 46.367 | 32.735 | 65.774 | 1.00 | 20.54 | AAAA |
| ATOM | 911 | CB | GLU | 116 | 45.744 | 34.044 | 65.320 | 1.00 | 18.40 | AAAA |
| ATOM | 912 | CG | GLU | 116 | 46.562 | 34.765 | 64.279 | 1.00 | 19.76 | AAAA |
| ATOM | 913 | CD | GLU | 116 | 47.985 | 34.998 | 64.756 | 1.00 | 27.24 | AAAA |
| ATOM | 914 | OE1 | GLU | 116 | 48.164 | 35.630 | 65.815 | 1.00 | 18.44 | AAAA |
| ATOM | 915 | OE2 | GLU | 116 | 48.919 | 34.543 | 64.078 | 1.00 | 23.17 | AAAA |
| ATOM | 916 | C | GLU | 116 | 45.682 | 32.253 | 67.034 | 1.00 | 25.39 | AAAA |
| ATOM | 917 | O | GLU | 116 | 46.207 | 32.427 | 68.137 | 1.00 | 22.87 | AAAA |
| ATOM | 918 | N | PHE | 117 | 44.510 | 31.647 | 66.872 | 1.00 | 18.78 | AAAA |
| ATOM | 919 | CA | PHE | 117 | 43.778 | 31.139 | 68.019 | 1.00 | 22.11 | AAAA |
| ATOM | 920 | CB | PHE | 117 | 42.451 | 30.530 | 67.581 | 1.00 | 23.14 | AAAA |
| ATOM | 921 | CG | PHE | 117 | 41.603 | 30.054 | 68.728 | 1.00 | 24.06 | AAAA |
| ATOM | 922 | CD1 | PHE | 117 | 40.880 | 30.961 | 69.493 | 1.00 | 19.67 | AAAA |
| ATOM | 923 | CD2 | PHE | 117 | 41.559 | 28.701 | 69.066 | 1.00 | 24.08 | AAAA |
| ATOM | 924 | CE1 | PHE | 117 | 40.115 | 30.531 | 70.586 | 1.00 | 23.68 | AAAA |

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| | | | | | | | | | | |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 925 | CE2 | PHE | 117 | 40.799 | 28.262 | 70.156 | 1.00 | 24.04 | AAAA |
| ATOM | 926 | CZ | PHE | 117 | 40.078 | 29.179 | 70.915 | 1.00 | 19.62 | AAAA |
| ATOM | 927 | C | PHE | 117 | 44.587 | 30.068 | 68.747 | 1.00 | 23.87 | AAAA |
| ATOM | 928 | O | PHE | 117 | 44.613 | 30.031 | 69.979 | 1.00 | 24.40 | AAAA |
| ATOM | 929 | N | LEU | 118 | 45.238 | 29.194 | 67.981 | 1.00 | 21.09 | AAAA |
| ATOM | 930 | CA | LEU | 118 | 46.025 | 28.113 | 68.549 | 1.00 | 20.73 | AAAA |
| ATOM | 931 | CB | LEU | 118 | 46.358 | 27.075 | 67.480 | 1.00 | 17.90 | AAAA |
| ATOM | 932 | CG | LEU | 118 | 45.148 | 26.264 | 66.984 | 1.00 | 26.20 | AAAA |
| ATOM | 933 | CD1 | LEU | 118 | 45.591 | 25.288 | 65.924 | 1.00 | 34.23 | AAAA |
| ATOM | 934 | CD2 | LEU | 118 | 44.520 | 25.499 | 68.139 | 1.00 | 27.16 | AAAA |
| ATOM | 935 | C | LEU | 118 | 47.290 | 28.601 | 69.238 | 1.00 | 26.49 | AAAA |
| ATOM | 936 | O | LEU | 118 | 47.908 | 27.856 | 69.996 | 1.00 | 26.34 | AAAA |
| ATOM | 937 | N | LYS | 119 | 47.672 | 29.848 | 68.975 | 1.00 | 28.92 | AAAA |
| ATOM | 938 | CA | LYS | 119 | 48.835 | 30.459 | 69.624 | 1.00 | 28.53 | AAAA |
| ATOM | 939 | CB | LYS | 119 | 49.392 | 31.616 | 68.805 | 1.00 | 30.15 | AAAA |
| ATOM | 940 | CG | LYS | 119 | 49.915 | 31.267 | 67.437 | 1.00 | 35.14 | AAAA |
| ATOM | 941 | CD | LYS | 119 | 50.291 | 32.549 | 66.716 | 1.00 | 28.98 | AAAA |
| ATOM | 942 | CE | LYS | 119 | 50.905 | 32.262 | 65.380 | 1.00 | 31.07 | AAAA |
| ATOM | 943 | NZ | LYS | 119 | 51.195 | 33.551 | 64.745 | 1.00 | 22.46 | AAAA |
| ATOM | 944 | C | LYS | 119 | 48.335 | 31.053 | 70.932 | 1.00 | 35.74 | AAAA |
| ATOM | 945 | O | LYS | 119 | 49.117 | 31.541 | 71.750 | 1.00 | 27.10 | AAAA |
| ATOM | 946 | N | GLY | 120 | 47.018 | 31.050 | 71.103 | 1.00 | 25.20 | AAAA |
| ATOM | 947 | CA | GLY | 120 | 46.445 | 31.605 | 72.309 | 1.00 | 30.18 | AAAA |
| ATOM | 948 | C | GLY | 120 | 45.913 | 33.007 | 72.122 | 1.00 | 31.91 | AAAA |
| ATOM | 949 | O | GLY | 120 | 45.540 | 33.665 | 73.094 | 1.00 | 34.76 | AAAA |
| ATOM | 950 | N | ASN | 121 | 45.889 | 33.495 | 70.887 | 1.00 | 20.56 | AAAA |
| ATOM | 951 | CA | ASN | 121 | 45.353 | 34.825 | 70.681 | 1.00 | 25.58 | AAAA |
| ATOM | 952 | CB | ASN | 121 | 46.278 | 35.634 | 69.785 | 1.00 | 29.99 | AAAA |
| ATOM | 953 | CG | ASN | 121 | 47.641 | 35.827 | 70.427 | 1.00 | 24.43 | AAAA |
| ATOM | 954 | OD1 | ASN | 121 | 48.396 | 34.874 | 70.588 | 1.00 | 54.63 | AAAA |
| ATOM | 955 | ND2 | ASN | 121 | 47.944 | 37.045 | 70.817 | 1.00 | 41.69 | AAAA |
| ATOM | 956 | C | ASN | 121 | 43.941 | 34.759 | 70.135 | 1.00 | 18.85 | AAAA |
| ATOM | 957 | O | ASN | 121 | 43.421 | 33.675 | 69.899 | 1.00 | 24.77 | AAAA |
| ATOM | 958 | N | VAL | 122 | 43.310 | 35.918 | 69.991 | 1.00 | 19.55 | AAAA |
| ATOM | 959 | CA | VAL | 122 | 41.936 | 35.994 | 69.499 | 1.00 | 22.90 | AAAA |
| ATOM | 960 | CB | VAL | 122 | 41.053 | 36.832 | 70.449 | 1.00 | 31.47 | AAAA |
| ATOM | 961 | CG1 | VAL | 122 | 39.649 | 37.006 | 69.851 | 1.00 | 31.52 | AAAA |
| ATOM | 962 | CG2 | VAL | 122 | 40.986 | 36.154 | 71.810 | 1.00 | 32.50 | AAAA |
| ATOM | 963 | C | VAL | 122 | 41.953 | 36.632 | 68.130 | 1.00 | 16.87 | AAAA |
| ATOM | 964 | O | VAL | 122 | 42.518 | 37.710 | 67.938 | 1.00 | 24.08 | AAAA |
| ATOM | 965 | N | ALA | 123 | 41.321 | 35.983 | 67.159 | 1.00 | 18.67 | AAAA |
| ATOM | 966 | CA | ALA | 123 | 41.360 | 36.532 | 65.821 | 1.00 | 10.18 | AAAA |
| ATOM | 967 | CB | ALA | 123 | 42.346 | 35.743 | 64.990 | 1.00 | 19.04 | AAAA |
| ATOM | 968 | C | ALA | 123 | 40.000 | 36.551 | 65.131 | 1.00 | 13.72 | AAAA |
| ATOM | 969 | O | ALA | 123 | 39.108 | 35.761 | 65.439 | 1.00 | 20.78 | AAAA |
| ATOM | 970 | N | PHE | 124 | 39.871 | 37.457 | 64.180 | 1.00 | 12.92 | AAAA |
| ATOM | 971 | CA | PHE | 124 | 38.649 | 37.610 | 63.401 | 1.00 | 14.67 | AAAA |
| ATOM | 972 | CB | PHE | 124 | 37.904 | 38.878 | 63.856 | 1.00 | 14.67 | AAAA |
| ATOM | 973 | CG | PHE | 124 | 36.660 | 39.209 | 63.049 | 1.00 | 20.28 | AAAA |
| ATOM | 974 | CD1 | PHE | 124 | 35.811 | 38.209 | 62.587 | 1.00 | 18.56 | AAAA |
| ATOM | 975 | CD2 | PHE | 124 | 36.286 | 40.545 | 62.843 | 1.00 | 19.53 | AAAA |
| ATOM | 976 | CE1 | PHE | 124 | 34.609 | 38.532 | 61.937 | 1.00 | 18.75 | AAAA |
| ATOM | 977 | CE2 | PHE | 124 | 35.072 | 40.875 | 62.193 | 1.00 | 20.18 | AAAA |
| ATOM | 978 | CZ | PHE | 124 | 34.242 | 39.867 | 61.744 | 1.00 | 21.57 | AAAA |
| ATOM | 979 | C | PHE | 124 | 39.016 | 37.712 | 61.930 | 1.00 | 22.60 | AAAA |
| ATOM | 980 | O | PHE | 124 | 39.823 | 38.558 | 61.535 | 1.00 | 19.22 | AAAA |
| ATOM | 981 | N | ASN | 125 | 38.449 | 36.820 | 61.126 | 1.00 | 19.39 | AAAA |
| ATOM | 982 | CA | ASN | 125 | 38.651 | 36.858 | 59.691 | 1.00 | 16.80 | AAAA |
| ATOM | 983 | CB | ASN | 125 | 39.122 | 35.507 | 59.150 | 1.00 | 15.71 | AAAA |
| ATOM | 984 | CG | ASN | 125 | 39.063 | 35.469 | 57.649 | 1.00 | 12.84 | AAAA |
| ATOM | 985 | OD1 | ASN | 125 | 39.216 | 36.508 | 57.006 | 1.00 | 14.91 | AAAA |
| ATOM | 986 | ND2 | ASN | 125 | 38.853 | 34.272 | 57.065 | 1.00 | 16.21 | AAAA |
| ATOM | 987 | C | ASN | 125 | 37.315 | 37.210 | 59.038 | 1.00 | 16.22 | AAAA |
| ATOM | 988 | O | ASN | 125 | 36.502 | 36.330 | 58.755 | 1.00 | 15.28 | AAAA |
| ATOM | 989 | N | PRO | 126 | 37.071 | 38.502 | 58.775 | 1.00 | 14.84 | AAAA |
| ATOM | 990 | CD | PRO | 126 | 37.908 | 39.684 | 59.052 | 1.00 | 18.10 | AAAA |

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Figure 16-16

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 991 | CA | PRO | 126 | 35.811 | 38.910 | 58.156 | 1.00 | 17.33 | AAAA |
| ATOM | 992 | CB | PRO | 126 | 35.912 | 40.434 | 58.177 | 1.00 | 16.32 | AAAA |
| ATOM | 993 | CG | PRO | 126 | 37.416 | 40.655 | 58.008 | 1.00 | 20.95 | AAAA |
| ATOM | 994 | C | PRO | 126 | 35.549 | 38.359 | 56.752 | 1.00 | 13.78 | AAAA |
| ATOM | 995 | O | PRO | 126 | 34.404 | 38.291 | 56.322 | 1.00 | 17.03 | AAAA |
| ATOM | 996 | N | ALA | 127 | 36.607 | 37.972 | 56.042 | 1.00 | 14.57 | AAAA |
| ATOM | 997 | CA | ALA | 127 | 36.463 | 37.443 | 54.691 | 1.00 | 17.37 | AAAA |
| ATOM | 998 | CB | ALA | 127 | 37.816 | 37.540 | 53.930 | 1.00 | 14.48 | AAAA |
| ATOM | 999 | C | ALA | 127 | 35.982 | 35.998 | 54.702 | 1.00 | 19.77 | AAAA |
| ATOM | 1000 | O | ALA | 127 | 35.490 | 35.500 | 53.688 | 1.00 | 15.62 | AAAA |
| ATOM | 1001 | N | GLY | 128 | 36.111 | 35.339 | 55.849 | 1.00 | 13.54 | AAAA |
| ATOM | 1002 | CA | GLY | 128 | 35.725 | 33.939 | 55.971 | 1.00 | 13.53 | AAAA |
| ATOM | 1003 | C | GLY | 128 | 34.234 | 33.679 | 56.101 | 1.00 | 14.49 | AAAA |
| ATOM | 1004 | O | GLY | 128 | 33.414 | 34.585 | 56.017 | 1.00 | 15.65 | AAAA |
| ATOM | 1005 | N | GLY | 129 | 33.883 | 32.420 | 56.314 | 1.00 | 13.35 | AAAA |
| ATOM | 1006 | CA | GLY | 129 | 32.487 | 32.058 | 56.446 | 1.00 | 16.28 | AAAA |
| ATOM | 1007 | C | GLY | 129 | 31.754 | 31.831 | 55.130 | 1.00 | 15.69 | AAAA |
| ATOM | 1008 | O | GLY | 129 | 30.543 | 32.021 | 55.072 | 1.00 | 16.10 | AAAA |
| ATOM | 1009 | N | MET | 130 | 32.479 | 31.448 | 54.079 | 1.00 | 15.00 | AAAA |
| ATOM | 1010 | CA | MET | 130 | 31.879 | 31.163 | 52.757 | 1.00 | 13.35 | AAAA |
| ATOM | 1011 | CB | MET | 130 | 32.969 | 31.215 | 51.689 | 1.00 | 12.20 | AAAA |
| ATOM | 1012 | CG | MET | 130 | 33.680 | 32.573 | 51.731 | 1.00 | 17.03 | AAAA |
| ATOM | 1013 | SD | MET | 130 | 34.863 | 32.877 | 50.425 | 1.00 | 15.41 | AAAA |
| ATOM | 1014 | CE | MET | 130 | 33.752 | 32.973 | 49.073 | 1.00 | 46.82 | AAAA |
| ATOM | 1015 | C | MET | 130 | 31.296 | 29.756 | 52.885 | 1.00 | 12.49 | AAAA |
| ATOM | 1016 | O | MET | 130 | 31.785 | 28.789 | 52.297 | 1.00 | 19.54 | AAAA |
| ATOM | 1017 | N | HIS | 131 | 30.188 | 29.695 | 53.617 | 1.00 | 16.24 | AAAA |
| ATOM | 1018 | CA | HIS | 131 | 29.556 | 28.448 | 54.014 | 1.00 | 13.80 | AAAA |
| ATOM | 1019 | CB | HIS | 131 | 28.772 | 28.694 | 55.316 | 1.00 | 15.91 | AAAA |
| ATOM | 1020 | CG | HIS | 131 | 27.606 | 29.625 | 55.175 | 1.00 | 13.08 | AAAA |
| ATOM | 1021 | CD2 | HIS | 131 | 26.712 | 30.063 | 56.096 | 1.00 | 12.46 | AAAA |
| ATOM | 1022 | ND1 | HIS | 131 | 27.225 | 30.190 | 53.976 | 1.00 | 22.48 | AAAA |
| ATOM | 1023 | CE1 | HIS | 131 | 26.148 | 30.936 | 54.166 | 1.00 | 16.56 | AAAA |
| ATOM | 1024 | NE2 | HIS | 131 | 25.817 | 30.875 | 55.442 | 1.00 | 23.56 | AAAA |
| ATOM | 1025 | C | HIS | 131 | 28.673 | 27.663 | 53.066 | 1.00 | 13.69 | AAAA |
| ATOM | 1026 | O | HIS | 131 | 28.125 | 26.658 | 53.470 | 1.00 | 17.21 | AAAA |
| ATOM | 1027 | N | HIS | 132 | 28.523 | 28.115 | 51.830 | 1.00 | 14.51 | AAAA |
| ATOM | 1028 | CA | HIS | 132 | 27.669 | 27.400 | 50.887 | 1.00 | 20.19 | AAAA |
| ATOM | 1029 | CB | HIS | 132 | 26.863 | 28.416 | 50.054 | 1.00 | 17.26 | AAAA |
| ATOM | 1030 | CG | HIS | 132 | 25.748 | 29.070 | 50.810 | 1.00 | 16.85 | AAAA |
| ATOM | 1031 | CD2 | HIS | 132 | 24.787 | 28.542 | 51.604 | 1.00 | 13.74 | AAAA |
| ATOM | 1032 | ND1 | HIS | 132 | 25.497 | 30.424 | 50.756 | 1.00 | 24.80 | AAAA |
| ATOM | 1033 | CE1 | HIS | 132 | 24.429 | 30.700 | 51.486 | 1.00 | 12.68 | AAAA |
| ATOM | 1034 | NE2 | HIS | 132 | 23.980 | 29.576 | 52.010 | 1.00 | 28.65 | AAAA |
| ATOM | 1035 | C | HIS | 132 | 28.372 | 26.412 | 49.946 | 1.00 | 16.89 | AAAA |
| ATOM | 1036 | O | HIS | 132 | 27.731 | 25.487 | 49.460 | 1.00 | 14.58 | AAAA |
| ATOM | 1037 | N | ALA | 133 | 29.669 | 26.580 | 49.689 | 1.00 | 16.79 | AAAA |
| ATOM | 1038 | CA | ALA | 133 | 30.338 | 25.680 | 48.740 | 1.00 | 13.76 | AAAA |
| ATOM | 1039 | CB | ALA | 133 | 31.738 | 26.194 | 48.412 | 1.00 | 14.95 | AAAA |
| ATOM | 1040 | C | ALA | 133 | 30.418 | 24.219 | 49.179 | 1.00 | 18.80 | AAAA |
| ATOM | 1041 | O | ALA | 133 | 30.557 | 23.939 | 50.355 | 1.00 | 16.86 | AAAA |
| ATOM | 1042 | N | PHE | 134 | 30.306 | 23.306 | 48.209 | 1.00 | 13.76 | AAAA |
| ATOM | 1043 | CA | PHE | 134 | 30.378 | 21.868 | 48.451 | 1.00 | 19.77 | AAAA |
| ATOM | 1044 | CB | PHE | 134 | 29.311 | 21.132 | 47.620 | 1.00 | 15.59 | AAAA |
| ATOM | 1045 | CG | PHE | 134 | 27.917 | 21.525 | 47.975 | 1.00 | 17.22 | AAAA |
| ATOM | 1046 | CD1 | PHE | 134 | 27.135 | 22.259 | 47.091 | 1.00 | 17.88 | AAAA |
| ATOM | 1047 | CD2 | PHE | 134 | 27.392 | 21.187 | 49.222 | 1.00 | 21.68 | AAAA |
| ATOM | 1048 | CE1 | PHE | 134 | 25.836 | 22.653 | 47.445 | 1.00 | 23.07 | AAAA |
| ATOM | 1049 | CE2 | PHE | 134 | 26.099 | 21.578 | 49.585 | 1.00 | 17.64 | AAAA |
| ATOM | 1050 | CZ | PHE | 134 | 25.323 | 22.308 | 48.696 | 1.00 | 19.71 | AAAA |
| ATOM | 1051 | C | PHE | 134 | 31.763 | 21.354 | 48.098 | 1.00 | 14.76 | AAAA |
| ATOM | 1052 | O | PHE | 134 | 32.547 | 22.049 | 47.442 | 1.00 | 18.05 | AAAA |
| ATOM | 1053 | N | LYS | 135 | 32.060 | 20.124 | 48.515 | 1.00 | 16.37 | AAAA |
| ATOM | 1054 | CA | LYS | 135 | 33.369 | 19.551 | 48.269 | 1.00 | 16.24 | AAAA |
| ATOM | 1055 | CB | LYS | 135 | 33.360 | 18.070 | 48.699 | 1.00 | 21.29 | AAAA |
| ATOM | 1056 | CG | LYS | 135 | 34.640 | 17.300 | 48.400 | 1.00 | 30.43 | AAAA |

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| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1057 | CD | LYS | 135 | 34.597 | 15.867 | 48.977 | 1.00 | 30.26 | AAAA |
| ATOM | 1058 | CE | LYS | 135 | 34.862 | 15.805 | 50.486 | 1.00 | 35.01 | AAAA |
| ATOM | 1059 | NZ | LYS | 135 | 36.304 | 16.023 | 50.895 | 1.00 | 20.61 | AAAA |
| ATOM | 1060 | C | LYS | 135 | 33.854 | 19.687 | 46.836 | 1.00 | 16.60 | AAAA |
| ATOM | 1061 | O | LYS | 135 | 35.020 | 20.020 | 46.584 | 1.00 | 17.24 | AAAA |
| ATOM | 1062 | N | SER | 136 | 32.944 | 19.483 | 45.893 | 1.00 | 18.01 | AAAA |
| ATOM | 1063 | CA | SER | 136 | 33.301 | 19.528 | 44.490 | 1.00 | 15.26 | AAAA |
| ATOM | 1064 | CB | SER | 136 | 33.339 | 18.094 | 43.940 | 1.00 | 18.07 | AAAA |
| ATOM | 1065 | OG | SER | 136 | 34.135 | 17.261 | 44.762 | 1.00 | 22.22 | AAAA |
| ATOM | 1066 | C | SER | 136 | 32.345 | 20.355 | 43.658 | 1.00 | 15.40 | AAAA |
| ATOM | 1067 | O | SER | 136 | 32.162 | 20.071 | 42.475 | 1.00 | 18.77 | AAAA |
| ATOM | 1068 | N | ARG | 137 | 31.754 | 21.401 | 44.237 | 1.00 | 19.71 | AAAA |
| ATOM | 1069 | CA | ARG | 137 | 30.805 | 22.216 | 43.482 | 1.00 | 17.29 | AAAA |
| ATOM | 1070 | CB | ARG | 137 | 29.481 | 21.448 | 43.366 | 1.00 | 24.19 | AAAA |
| ATOM | 1071 | CG | ARG | 137 | 28.290 | 22.273 | 42.937 | 1.00 | 32.56 | AAAA |
| ATOM | 1072 | CD | ARG | 137 | 27.026 | 21.424 | 42.980 | 1.00 | 47.98 | AAAA |
| ATOM | 1073 | NE | ARG | 137 | 26.951 | 20.493 | 41.862 | 1.00 | 50.95 | AAAA |
| ATOM | 1074 | CZ | ARG | 137 | 26.392 | 20.781 | 40.691 | 1.00 | 50.38 | AAAA |
| ATOM | 1075 | NH1 | ARG | 137 | 25.854 | 21.976 | 40.485 | 1.00 | 45.26 | AAAA |
| ATOM | 1076 | NH2 | ARG | 137 | 26.375 | 19.876 | 39.722 | 1.00 | 55.31 | AAAA |
| ATOM | 1077 | C | ARG | 137 | 30.537 | 23.595 | 44.095 | 1.00 | 16.14 | AAAA |
| ATOM | 1078 | O | ARG | 137 | 30.439 | 23.711 | 45.308 | 1.00 | 16.88 | AAAA |
| ATOM | 1079 | N | ALA | 138 | 30.395 | 24.621 | 43.252 | 1.00 | 18.07 | AAAA |
| ATOM | 1080 | CA | ALA | 138 | 30.117 | 25.976 | 43.735 | 1.00 | 21.48 | AAAA |
| ATOM | 1081 | CB | ALA | 138 | 30.460 | 27.024 | 42.631 | 1.00 | 16.55 | AAAA |
| ATOM | 1082 | C | ALA | 138 | 28.642 | 26.090 | 44.135 | 1.00 | 21.04 | AAAA |
| ATOM | 1083 | O | ALA | 138 | 27.798 | 25.339 | 43.641 | 1.00 | 18.97 | AAAA |
| ATOM | 1084 | N | ASN | 139 | 28.321 | 27.019 | 45.029 | 1.00 | 13.83 | AAAA |
| ATOM | 1085 | CA | ASN | 139 | 26.952 | 27.158 | 45.468 | 1.00 | 12.92 | AAAA |
| ATOM | 1086 | CB | ASN | 139 | 26.566 | 25.899 | 46.274 | 1.00 | 13.14 | AAAA |
| ATOM | 1087 | CG | ASN | 139 | 25.162 | 25.961 | 46.832 | 1.00 | 20.34 | AAAA |
| ATOM | 1088 | OD1 | ASN | 139 | 24.186 | 26.068 | 46.086 | 1.00 | 19.76 | AAAA |
| ATOM | 1089 | ND2 | ASN | 139 | 25.048 | 25.881 | 48.157 | 1.00 | 16.36 | AAAA |
| ATOM | 1090 | C | ASN | 139 | 26.756 | 28.409 | 46.315 | 1.00 | 20.92 | AAAA |
| ATOM | 1091 | O | ASN | 139 | 27.603 | 28.738 | 47.148 | 1.00 | 16.81 | AAAA |
| ATOM | 1092 | N | GLY | 140 | 25.644 | 29.105 | 46.086 | 1.00 | 19.30 | AAAA |
| ATOM | 1093 | CA | GLY | 140 | 25.330 | 30.295 | 46.864 | 1.00 | 21.34 | AAAA |
| ATOM | 1094 | C | GLY | 140 | 26.393 | 31.378 | 46.888 | 1.00 | 20.19 | AAAA |
| ATOM | 1095 | O | GLY | 140 | 26.653 | 31.968 | 47.943 | 1.00 | 18.77 | AAAA |
| ATOM | 1096 | N | PHE | 141 | 26.996 | 31.649 | 45.733 | 1.00 | 15.52 | AAAA |
| ATOM | 1097 | CA | PHE | 141 | 28.034 | 32.675 | 45.600 | 1.00 | 20.71 | AAAA |
| ATOM | 1098 | CB | PHE | 141 | 27.711 | 33.952 | 46.388 | 1.00 | 20.03 | AAAA |
| ATOM | 1099 | CG | PHE | 141 | 26.355 | 34.544 | 46.127 | 1.00 | 28.32 | AAAA |
| ATOM | 1100 | CD1 | PHE | 141 | 25.855 | 35.526 | 46.997 | 1.00 | 24.25 | AAAA |
| ATOM | 1101 | CD2 | PHE | 141 | 25.589 | 34.170 | 45.029 | 1.00 | 30.11 | AAAA |
| ATOM | 1102 | CE1 | PHE | 141 | 24.628 | 36.116 | 46.775 | 1.00 | 25.94 | AAAA |
| ATOM | 1103 | CE2 | PHE | 141 | 24.346 | 34.766 | 44.801 | 1.00 | 21.61 | AAAA |
| ATOM | 1104 | CZ | PHE | 141 | 23.870 | 35.741 | 45.677 | 1.00 | 24.41 | AAAA |
| ATOM | 1105 | C | PHE | 141 | 29.357 | 32.188 | 46.158 | 1.00 | 14.45 | AAAA |
| ATOM | 1106 | O | PHE | 141 | 30.336 | 32.914 | 46.111 | 1.00 | 16.39 | AAAA |
| ATOM | 1107 | N | CYS | 142 | 29.389 | 30.982 | 46.716 | 1.00 | 16.77 | AAAA |
| ATOM | 1108 | CA | CYS | 142 | 30.629 | 30.466 | 47.285 | 1.00 | 17.71 | AAAA |
| ATOM | 1109 | CB | CYS | 142 | 30.347 | 29.845 | 48.659 | 1.00 | 13.95 | AAAA |
| ATOM | 1110 | SG | CYS | 142 | 29.606 | 30.985 | 49.846 | 1.00 | 16.63 | AAAA |
| ATOM | 1111 | C | CYS | 142 | 31.313 | 29.421 | 46.401 | 1.00 | 18.09 | AAAA |
| ATOM | 1112 | O | CYS | 142 | 30.647 | 28.527 | 45.856 | 1.00 | 16.60 | AAAA |
| ATOM | 1113 | N | TYR | 143 | 32.639 | 29.539 | 46.272 | 1.00 | 12.50 | AAAA |
| ATOM | 1114 | CA | TYR | 143 | 33.429 | 28.603 | 45.478 | 1.00 | 15.32 | AAAA |
| ATOM | 1115 | CB | TYR | 143 | 34.333 | 29.322 | 44.473 | 1.00 | 13.07 | AAAA |
| ATOM | 1116 | CG | TYR | 143 | 33.614 | 30.338 | 43.612 | 1.00 | 15.80 | AAAA |
| ATOM | 1117 | CD1 | TYR | 143 | 33.396 | 31.636 | 44.071 | 1.00 | 15.48 | AAAA |
| ATOM | 1118 | CE1 | TYR | 143 | 32.740 | 32.589 | 43.270 | 1.00 | 11.99 | AAAA |
| ATOM | 1119 | CD2 | TYR | 143 | 33.157 | 29.999 | 42.336 | 1.00 | 14.60 | AAAA |
| ATOM | 1120 | CE2 | TYR | 143 | 32.501 | 30.935 | 41.532 | 1.00 | 10.74 | AAAA |
| ATOM | 1121 | CZ | TYR | 143 | 32.301 | 32.229 | 42.008 | 1.00 | 20.89 | AAAA |
| ATOM | 1122 | OH | TYR | 143 | 31.698 | 33.177 | 41.208 | 1.00 | 18.87 | AAAA |

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| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1123 | C | TYR | 143 | 34.310 | 27.723 | 46.358 | 1.00 | 17.35 | AAAA |
| ATOM | 1124 | O | TYR | 143 | 34.581 | 26.574 | 46.013 | 1.00 | 16.67 | AAAA |
| ATOM | 1125 | N | ILE | 144 | 34.763 | 28.262 | 47.489 | 1.00 | 14.93 | AAAA |
| ATOM | 1126 | CA | ILE | 144 | 35.599 | 27.500 | 48.408 | 1.00 | 14.17 | AAAA |
| ATOM | 1127 | CB | ILE | 144 | 37.018 | 28.069 | 48.440 | 1.00 | 14.87 | AAAA |
| ATOM | 1128 | CG2 | ILE | 144 | 37.864 | 27.332 | 49.474 | 1.00 | 13.55 | AAAA |
| ATOM | 1129 | CG1 | ILE | 144 | 37.611 | 28.027 | 47.021 | 1.00 | 16.98 | AAAA |
| ATOM | 1130 | CD1 | ILE | 144 | 39.052 | 28.537 | 46.901 | 1.00 | 17.42 | AAAA |
| ATOM | 1131 | C | ILE | 144 | 34.959 | 27.615 | 49.788 | 1.00 | 17.22 | AAAA |
| ATOM | 1132 | O | ILE | 144 | 34.606 | 28.716 | 50.220 | 1.00 | 14.72 | AAAA |
| ATOM | 1133 | N | ASN | 145 | 34.798 | 26.486 | 50.474 | 1.00 | 13.46 | AAAA |
| ATOM | 1134 | CA | ASN | 145 | 34.170 | 26.493 | 51.797 | 1.00 | 16.09 | AAAA |
| ATOM | 1135 | CB | ASN | 145 | 33.401 | 25.178 | 51.988 | 1.00 | 14.50 | AAAA |
| ATOM | 1136 | CG | ASN | 145 | 32.428 | 25.239 | 53.148 | 1.00 | 15.64 | AAAA |
| ATOM | 1137 | OD1 | ASN | 145 | 32.800 | 25.587 | 54.263 | 1.00 | 14.97 | AAAA |
| ATOM | 1138 | ND2 | ASN | 145 | 31.170 | 24.916 | 52.882 | 1.00 | 16.74 | AAAA |
| ATOM | 1139 | C | ASN | 145 | 35.266 | 26.639 | 52.873 | 1.00 | 15.04 | AAAA |
| ATOM | 1140 | O | ASN | 145 | 35.812 | 25.637 | 53.338 | 1.00 | 15.72 | AAAA |
| ATOM | 1141 | N | ASN | 146 | 35.599 | 27.865 | 53.282 | 1.00 | 12.34 | AAAA |
| ATOM | 1142 | CA | ASN | 146 | 36.685 | 28.006 | 54.262 | 1.00 | 15.31 | AAAA |
| ATOM | 1143 | CB | ASN | 146 | 37.161 | 29.464 | 54.354 | 1.00 | 15.81 | AAAA |
| ATOM | 1144 | CG | ASN | 146 | 36.101 | 30.396 | 54.865 | 1.00 | 15.25 | AAAA |
| ATOM | 1145 | OD1 | ASN | 146 | 36.113 | 30.757 | 56.034 | 1.00 | 13.57 | AAAA |
| ATOM | 1146 | ND2 | ASN | 146 | 35.156 | 30.775 | 53.996 | 1.00 | 10.85 | AAAA |
| ATOM | 1147 | C | ASN | 146 | 36.306 | 27.400 | 55.613 | 1.00 | 13.04 | AAAA |
| ATOM | 1148 | O | ASN | 146 | 37.160 | 26.865 | 56.314 | 1.00 | 14.76 | AAAA |
| ATOM | 1149 | N | PRO | 147 | 35.025 | 27.489 | 56.016 | 1.00 | 14.28 | AAAA |
| ATOM | 1150 | CD | PRO | 147 | 33.817 | 28.175 | 55.515 | 1.00 | 7.62 | AAAA |
| ATOM | 1151 | CA | PRO | 147 | 34.750 | 26.843 | 57.307 | 1.00 | 13.51 | AAAA |
| ATOM | 1152 | CB | PRO | 147 | 33.251 | 27.058 | 57.482 | 1.00 | 14.44 | AAAA |
| ATOM | 1153 | CG | PRO | 147 | 33.056 | 28.436 | 56.827 | 1.00 | 12.32 | AAAA |
| ATOM | 1154 | C | PRO | 147 | 35.118 | 25.330 | 57.278 | 1.00 | 18.86 | AAAA |
| ATOM | 1155 | O | PRO | 147 | 35.678 | 24.796 | 58.251 | 1.00 | 16.24 | AAAA |
| ATOM | 1156 | N | ALA | 148 | 34.818 | 24.642 | 56.171 | 1.00 | 15.01 | AAAA |
| ATOM | 1157 | CA | ALA | 148 | 35.122 | 23.200 | 56.080 | 1.00 | 15.58 | AAAA |
| ATOM | 1158 | CB | ALA | 148 | 34.402 | 22.561 | 54.882 | 1.00 | 12.93 | AAAA |
| ATOM | 1159 | C | ALA | 148 | 36.624 | 22.956 | 55.984 | 1.00 | 14.94 | AAAA |
| ATOM | 1160 | O | ALA | 148 | 37.138 | 21.999 | 56.560 | 1.00 | 14.69 | AAAA |
| ATOM | 1161 | N | VAL | 149 | 37.328 | 23.817 | 55.263 | 1.00 | 12.49 | AAAA |
| ATOM | 1162 | CA | VAL | 149 | 38.778 | 23.708 | 55.163 | 1.00 | 15.31 | AAAA |
| ATOM | 1163 | CB | VAL | 149 | 39.364 | 24.797 | 54.243 | 1.00 | 14.77 | AAAA |
| ATOM | 1164 | CG1 | VAL | 149 | 40.899 | 24.870 | 54.369 | 1.00 | 14.68 | AAAA |
| ATOM | 1165 | CG2 | VAL | 149 | 38.981 | 24.501 | 52.808 | 1.00 | 12.50 | AAAA |
| ATOM | 1166 | C | VAL | 149 | 39.323 | 23.887 | 56.572 | 1.00 | 20.14 | AAAA |
| ATOM | 1167 | O | VAL | 149 | 40.172 | 23.109 | 57.028 | 1.00 | 17.32 | AAAA |
| ATOM | 1168 | N | GLY | 150 | 38.815 | 24.899 | 57.271 | 1.00 | 15.45 | AAAA |
| ATOM | 1169 | CA | GLY | 150 | 39.284 | 25.168 | 58.622 | 1.00 | 20.96 | AAAA |
| ATOM | 1170 | C | GLY | 150 | 39.030 | 24.053 | 59.621 | 1.00 | 24.16 | AAAA |
| ATOM | 1171 | O | GLY | 150 | 39.888 | 23.738 | 60.458 | 1.00 | 19.50 | AAAA |
| ATOM | 1172 | N | ILE | 151 | 37.842 | 23.465 | 59.557 | 1.00 | 16.67 | AAAA |
| ATOM | 1173 | CA | ILE | 151 | 37.490 | 22.375 | 60.461 | 1.00 | 19.56 | AAAA |
| ATOM | 1174 | CB | ILE | 151 | 35.992 | 22.052 | 60.348 | 1.00 | 16.46 | AAAA |
| ATOM | 1175 | CG2 | ILE | 151 | 35.667 | 20.709 | 61.036 | 1.00 | 17.93 | AAAA |
| ATOM | 1176 | CG1 | ILE | 151 | 35.180 | 23.209 | 60.959 | 1.00 | 12.31 | AAAA |
| ATOM | 1177 | CD1 | ILE | 151 | 33.686 | 23.123 | 60.672 | 1.00 | 18.71 | AAAA |
| ATOM | 1178 | C | ILE | 151 | 38.352 | 21.148 | 60.164 | 1.00 | 22.66 | AAAA |
| ATOM | 1179 | O | ILE | 151 | 38.796 | 20.472 | 61.087 | 1.00 | 20.08 | AAAA |
| ATOM | 1180 | N | GLU | 152 | 38.599 | 20.861 | 58.888 | 1.00 | 19.71 | AAAA |
| ATOM | 1181 | CA | GLU | 152 | 39.434 | 19.718 | 58.533 | 1.00 | 13.85 | AAAA |
| ATOM | 1182 | CB | GLU | 152 | 39.362 | 19.437 | 57.033 | 1.00 | 20.21 | AAAA |
| ATOM | 1183 | CG | GLU | 152 | 38.033 | 18.833 | 56.624 | 1.00 | 22.16 | AAAA |
| ATOM | 1184 | CD | GLU | 152 | 37.838 | 17.430 | 57.166 | 1.00 | 26.94 | AAAA |
| ATOM | 1185 | OE1 | GLU | 152 | 36.720 | 16.906 | 57.035 | 1.00 | 25.03 | AAAA |
| ATOM | 1186 | OE2 | GLU | 152 | 38.800 | 16.846 | 57.708 | 1.00 | 24.95 | AAAA |
| ATOM | 1187 | C | GLU | 152 | 40.865 | 20.010 | 58.942 | 1.00 | 16.85 | AAAA |
| ATOM | 1188 | O | GLU | 152 | 41.629 | 19.110 | 59.289 | 1.00 | 19.25 | AAAA |

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Figure 16-19

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1189 | N | TYR | 153 | 41.228 | 21.290 | 58.931 | 1.00 | 14.74 | AAAA |
| ATOM | 1190 | CA | TYR | 153 | 42.574 | 21.672 | 59.350 | 1.00 | 17.71 | AAAA |
| ATOM | 1191 | CB | TYR | 153 | 42.757 | 23.193 | 59.179 | 1.00 | 13.26 | AAAA |
| ATOM | 1192 | CG | TYR | 153 | 44.059 | 23.727 | 59.729 | 1.00 | 16.36 | AAAA |
| ATOM | 1193 | CD1 | TYR | 153 | 45.234 | 23.726 | 58.967 | 1.00 | 18.41 | AAAA |
| ATOM | 1194 | CE1 | TYR | 153 | 46.438 | 24.219 | 59.511 | 1.00 | 21.03 | AAAA |
| ATOM | 1195 | CD2 | TYR | 153 | 44.115 | 24.220 | 61.028 | 1.00 | 21.16 | AAAA |
| ATOM | 1196 | CE2 | TYR | 153 | 45.288 | 24.705 | 61.570 | 1.00 | 19.76 | AAAA |
| ATOM | 1197 | CZ | TYR | 153 | 46.440 | 24.711 | 60.824 | 1.00 | 25.97 | AAAA |
| ATOM | 1198 | OH | TYR | 153 | 47.571 | 25.235 | 61.410 | 1.00 | 23.15 | AAAA |
| ATOM | 1199 | C | TYR | 153 | 42.712 | 21.274 | 60.828 | 1.00 | 20.00 | AAAA |
| ATOM | 1200 | O | TYR | 153 | 43.722 | 20.698 | 61.247 | 1.00 | 19.61 | AAAA |
| ATOM | 1201 | N | LEU | 154 | 41.683 | 21.569 | 61.616 | 1.00 | 17.78 | AAAA |
| ATOM | 1202 | CA | LEU | 154 | 41.698 | 21.239 | 63.042 | 1.00 | 17.26 | AAAA |
| ATOM | 1203 | CB | LEU | 154 | 40.511 | 21.913 | 63.744 | 1.00 | 20.44 | AAAA |
| ATOM | 1204 | CG | LEU | 154 | 40.636 | 23.434 | 63.942 | 1.00 | 19.57 | AAAA |
| ATOM | 1205 | CD1 | LEU | 154 | 39.277 | 24.046 | 64.309 | 1.00 | 22.48 | AAAA |
| ATOM | 1206 | CD2 | LEU | 154 | 41.692 | 23.709 | 65.044 | 1.00 | 20.84 | AAAA |
| ATOM | 1207 | C | LEU | 154 | 41.669 | 19.715 | 63.262 | 1.00 | 19.69 | AAAA |
| ATOM | 1208 | O | LEU | 154 | 42.357 | 19.191 | 64.149 | 1.00 | 22.91 | AAAA |
| ATOM | 1209 | N | ARG | 155 | 40.878 | 18.996 | 62.469 | 1.00 | 20.88 | AAAA |
| ATOM | 1210 | CA | ARG | 155 | 40.840 | 17.539 | 62.622 | 1.00 | 22.64 | AAAA |
| ATOM | 1211 | CB | ARG | 155 | 39.829 | 16.905 | 61.652 | 1.00 | 25.69 | AAAA |
| ATOM | 1212 | CG | ARG | 155 | 38.384 | 17.394 | 61.893 | 1.00 | 27.64 | AAAA |
| ATOM | 1213 | CD | ARG | 155 | 37.382 | 16.834 | 60.892 | 1.00 | 25.67 | AAAA |
| ATOM | 1214 | NE | ARG | 155 | 36.931 | 15.497 | 61.246 | 1.00 | 30.88 | AAAA |
| ATOM | 1215 | CZ | ARG | 155 | 36.135 | 14.753 | 60.488 | 1.00 | 36.28 | AAAA |
| ATOM | 1216 | NH1 | ARG | 155 | 35.705 | 15.218 | 59.318 | 1.00 | 26.96 | AAAA |
| ATOM | 1217 | NH2 | ARG | 155 | 35.737 | 13.562 | 60.923 | 1.00 | 27.33 | AAAA |
| ATOM | 1218 | C | ARG | 155 | 42.235 | 16.966 | 62.390 | 1.00 | 28.00 | AAAA |
| ATOM | 1219 | O | ARG | 155 | 42.674 | 16.070 | 63.119 | 1.00 | 28.05 | AAAA |
| ATOM | 1220 | N | LYS | 156 | 42.949 | 17.486 | 61.395 | 1.00 | 23.53 | AAAA |
| ATOM | 1221 | CA | LYS | 156 | 44.290 | 16.977 | 61.128 | 1.00 | 26.79 | AAAA |
| ATOM | 1222 | CB | LYS | 156 | 44.854 | 17.558 | 59.824 | 1.00 | 26.01 | AAAA |
| ATOM | 1223 | CG | LYS | 156 | 46.213 | 16.955 | 59.444 | 1.00 | 29.70 | AAAA |
| ATOM | 1224 | CD | LYS | 156 | 46.632 | 17.308 | 58.035 | 1.00 | 28.77 | AAAA |
| ATOM | 1225 | CE | LYS | 156 | 45.685 | 16.692 | 57.005 | 1.00 | 39.79 | AAAA |
| ATOM | 1226 | NZ | LYS | 156 | 45.671 | 15.192 | 57.058 | 1.00 | 36.33 | AAAA |
| ATOM | 1227 | C | LYS | 156 | 45.233 | 17.260 | 62.299 | 1.00 | 26.40 | AAAA |
| ATOM | 1228 | O | LYS | 156 | 46.188 | 16.511 | 62.529 | 1.00 | 26.19 | AAAA |
| ATOM | 1229 | N | LYS | 157 | 44.960 | 18.337 | 63.032 | 1.00 | 22.50 | AAAA |
| ATOM | 1230 | CA | LYS | 157 | 45.757 | 18.709 | 64.204 | 1.00 | 21.12 | AAAA |
| ATOM | 1231 | CB | LYS | 157 | 45.535 | 20.181 | 64.591 | 1.00 | 28.95 | AAAA |
| ATOM | 1232 | CG | LYS | 157 | 46.160 | 21.215 | 63.652 | 1.00 | 25.94 | AAAA |
| ATOM | 1233 | CD | LYS | 157 | 47.669 | 21.067 | 63.575 | 1.00 | 35.16 | AAAA |
| ATOM | 1234 | CE | LYS | 157 | 48.281 | 22.099 | 62.627 | 1.00 | 39.24 | AAAA |
| ATOM | 1235 | NZ | LYS | 157 | 49.742 | 21.869 | 62.406 | 1.00 | 40.01 | AAAA |
| ATOM | 1236 | C | LYS | 157 | 45.421 | 17.825 | 65.411 | 1.00 | 22.98 | AAAA |
| ATOM | 1237 | O | LYS | 157 | 46.085 | 17.903 | 66.444 | 1.00 | 27.77 | AAAA |
| ATOM | 1238 | N | GLY | 158 | 44.392 | 16.995 | 65.284 | 1.00 | 26.49 | AAAA |
| ATOM | 1239 | CA | GLY | 158 | 44.023 | 16.106 | 66.376 | 1.00 | 24.82 | AAAA |
| ATOM | 1240 | C | GLY | 158 | 42.771 | 16.459 | 67.161 | 1.00 | 33.13 | AAAA |
| ATOM | 1241 | O | GLY | 158 | 42.421 | 15.775 | 68.128 | 1.00 | 27.21 | AAAA |
| ATOM | 1242 | N | PHE | 159 | 42.085 | 17.529 | 66.781 | 1.00 | 27.47 | AAAA |
| ATOM | 1243 | CA | PHE | 159 | 40.866 | 17.861 | 67.502 | 1.00 | 24.15 | AAAA |
| ATOM | 1244 | CB | PHE | 159 | 40.410 | 19.285 | 67.186 | 1.00 | 27.53 | AAAA |
| ATOM | 1245 | CG | PHE | 159 | 41.264 | 20.343 | 67.827 | 1.00 | 27.26 | AAAA |
| ATOM | 1246 | CD1 | PHE | 159 | 42.439 | 20.785 | 67.220 | 1.00 | 28.12 | AAAA |
| ATOM | 1247 | CD2 | PHE | 159 | 40.926 | 20.842 | 69.076 | 1.00 | 21.10 | AAAA |
| ATOM | 1248 | CE1 | PHE | 159 | 43.264 | 21.714 | 67.866 | 1.00 | 26.24 | AAAA |
| ATOM | 1249 | CE2 | PHE | 159 | 41.738 | 21.768 | 69.736 | 1.00 | 26.07 | AAAA |
| ATOM | 1250 | CZ | PHE | 159 | 42.907 | 22.205 | 69.135 | 1.00 | 23.91 | AAAA |
| ATOM | 1251 | C | PHE | 159 | 39.792 | 16.854 | 67.120 | 1.00 | 28.02 | AAAA |
| ATOM | 1252 | O | PHE | 159 | 39.639 | 16.533 | 65.947 | 1.00 | 21.14 | AAAA |
| ATOM | 1253 | N | LYS | 160 | 39.056 | 16.361 | 68.110 | 1.00 | 24.79 | AAAA |
| ATOM | 1254 | CA | LYS | 160 | 38.011 | 15.366 | 67.881 | 1.00 | 24.26 | AAAA |

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Figure 16-20

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1255 | CB | LYS | 160 | 38.360 | 14.098 | 68.668 | 1.00 | 22.86 | AAAA |
| ATOM | 1256 | CG | LYS | 160 | 39.625 | 13.424 | 68.157 | 1.00 | 43.16 | AAAA |
| ATOM | 1257 | CD | LYS | 160 | 40.222 | 12.417 | 69.141 | 1.00 | 54.05 | AAAA |
| ATOM | 1258 | CE | LYS | 160 | 39.236 | 11.343 | 69.577 | 1.00 | 62.87 | AAAA |
| ATOM | 1259 | NZ | LYS | 160 | 38.154 | 11.890 | 70.446 | 1.00 | 68.11 | AAAA |
| ATOM | 1260 | C | LYS | 160 | 36.599 | 15.822 | 68.225 | 1.00 | 21.12 | AAAA |
| ATOM | 1261 | O | LYS | 160 | 35.632 | 15.672 | 68.051 | 1.00 | 22.43 | AAAA |
| ATOM | 1262 | N | ARG | 161 | 36.476 | 17.042 | 68.733 | 1.00 | 19.68 | AAAA |
| ATOM | 1263 | CA | ARG | 161 | 35.164 | 17.594 | 69.073 | 1.00 | 20.84 | AAAA |
| ATOM | 1264 | CB | ARG | 161 | 34.865 | 17.467 | 70.572 | 1.00 | 26.02 | AAAA |
| ATOM | 1265 | CG | ARG | 161 | 34.715 | 16.031 | 71.080 | 1.00 | 28.47 | AAAA |
| ATOM | 1266 | CD | ARG | 161 | 34.213 | 16.025 | 72.523 | 1.00 | 30.38 | AAAA |
| ATOM | 1267 | NE | ARG | 161 | 35.098 | 16.734 | 73.445 | 1.00 | 32.99 | AAAA |
| ATOM | 1268 | CZ | ARG | 161 | 36.272 | 16.278 | 73.883 | 1.00 | 40.49 | AAAA |
| ATOM | 1269 | NH1 | ARG | 161 | 36.724 | 15.094 | 73.489 | 1.00 | 31.49 | AAAA |
| ATOM | 1270 | NH2 | ARG | 161 | 37.003 | 17.014 | 74.712 | 1.00 | 38.54 | AAAA |
| ATOM | 1271 | C | ARG | 161 | 35.171 | 19.060 | 68.680 | 1.00 | 18.98 | AAAA |
| ATOM | 1272 | O | ARG | 161 | 35.552 | 19.932 | 69.460 | 1.00 | 23.57 | AAAA |
| ATOM | 1273 | N | ILE | 162 | 34.743 | 19.332 | 67.458 | 1.00 | 19.82 | AAAA |
| ATOM | 1274 | CA | ILE | 162 | 34.744 | 20.700 | 66.947 | 1.00 | 17.81 | AAAA |
| ATOM | 1275 | CB | ILE | 162 | 35.522 | 20.717 | 65.626 | 1.00 | 18.33 | AAAA |
| ATOM | 1276 | CG2 | ILE | 162 | 35.542 | 22.110 | 65.042 | 1.00 | 13.65 | AAAA |
| ATOM | 1277 | CG1 | ILE | 162 | 36.937 | 20.200 | 65.895 | 1.00 | 18.15 | AAAA |
| ATOM | 1278 | CD1 | ILE | 162 | 37.722 | 19.852 | 64.670 | 1.00 | 22.52 | AAAA |
| ATOM | 1279 | C | ILE | 162 | 33.316 | 21.184 | 66.724 | 1.00 | 14.71 | AAAA |
| ATOM | 1280 | O | ILE | 162 | 32.520 | 20.492 | 66.126 | 1.00 | 17.99 | AAAA |
| ATOM | 1281 | N | LEU | 163 | 32.996 | 22.374 | 67.217 | 1.00 | 16.93 | AAAA |
| ATOM | 1282 | CA | LEU | 163 | 31.653 | 22.902 | 67.061 | 1.00 | 20.73 | AAAA |
| ATOM | 1283 | CB | LEU | 163 | 31.115 | 23.376 | 68.421 | 1.00 | 18.45 | AAAA |
| ATOM | 1284 | CG | LEU | 163 | 29.846 | 24.236 | 68.463 | 1.00 | 19.99 | AAAA |
| ATOM | 1285 | CD1 | LEU | 163 | 28.657 | 23.408 | 67.975 | 1.00 | 15.66 | AAAA |
| ATOM | 1286 | CD2 | LEU | 163 | 29.609 | 24.751 | 69.870 | 1.00 | 18.74 | AAAA |
| ATOM | 1287 | C | LEU | 163 | 31.705 | 24.071 | 66.106 | 1.00 | 18.40 | AAAA |
| ATOM | 1288 | O | LEU | 163 | 32.607 | 24.889 | 66.188 | 1.00 | 18.65 | AAAA |
| ATOM | 1289 | N | TYR | 164 | 30.752 | 24.128 | 65.186 | 1.00 | 16.97 | AAAA |
| ATOM | 1290 | CA | TYR | 164 | 30.656 | 25.246 | 64.252 | 1.00 | 11.76 | AAAA |
| ATOM | 1291 | CB | TYR | 164 | 30.782 | 24.754 | 62.816 | 1.00 | 14.07 | AAAA |
| ATOM | 1292 | CG | TYR | 164 | 30.593 | 25.851 | 61.797 | 1.00 | 14.51 | AAAA |
| ATOM | 1293 | CD1 | TYR | 164 | 31.573 | 26.822 | 61.562 | 1.00 | 27.08 | AAAA |
| ATOM | 1294 | CE1 | TYR | 164 | 31.353 | 27.832 | 60.598 | 1.00 | 26.21 | AAAA |
| ATOM | 1295 | CD2 | TYR | 164 | 29.415 | 25.916 | 61.070 | 1.00 | 21.45 | AAAA |
| ATOM | 1296 | CE2 | TYR | 164 | 29.193 | 26.891 | 60.137 | 1.00 | 21.89 | AAAA |
| ATOM | 1297 | CZ | TYR | 164 | 30.148 | 27.839 | 59.896 | 1.00 | 16.35 | AAAA |
| ATOM | 1298 | OH | TYR | 164 | 29.857 | 28.764 | 58.913 | 1.00 | 27.44 | AAAA |
| ATOM | 1299 | C | TYR | 164 | 29.279 | 25.873 | 64.463 | 1.00 | 15.67 | AAAA |
| ATOM | 1300 | O | TYR | 164 | 28.760 | 25.177 | 64.455 | 1.00 | 16.07 | AAAA |
| ATOM | 1301 | N | ILE | 165 | 29.740 | 27.187 | 64.674 | 1.00 | 14.52 | AAAA |
| ATOM | 1302 | CA | ILE | 165 | 27.778 | 27.887 | 64.893 | 1.00 | 18.37 | AAAA |
| ATOM | 1303 | CB | ILE | 165 | 27.959 | 28.596 | 66.254 | 1.00 | 13.31 | AAAA |
| ATOM | 1304 | CG2 | ILE | 165 | 26.654 | 29.359 | 66.419 | 1.00 | 13.06 | AAAA |
| ATOM | 1305 | CG1 | ILE | 165 | 28.172 | 27.573 | 67.376 | 1.00 | 17.28 | AAAA |
| ATOM | 1306 | CD1 | ILE | 165 | 28.493 | 28.209 | 68.739 | 1.00 | 15.02 | AAAA |
| ATOM | 1307 | C | ILE | 165 | 27.853 | 28.926 | 63.779 | 1.00 | 20.75 | AAAA |
| ATOM | 1308 | O | ILE | 165 | 28.759 | 29.733 | 63.569 | 1.00 | 16.67 | AAAA |
| ATOM | 1309 | N | ASP | 166 | 26.725 | 28.901 | 63.084 | 1.00 | 15.37 | AAAA |
| ATOM | 1310 | CA | ASP | 166 | 26.503 | 29.779 | 61.942 | 1.00 | 15.63 | AAAA |
| ATOM | 1311 | CB | ASP | 166 | 26.276 | 28.885 | 60.698 | 1.00 | 12.31 | AAAA |
| ATOM | 1312 | CG | ASP | 166 | 26.279 | 29.666 | 59.393 | 1.00 | 16.37 | AAAA |
| ATOM | 1313 | OD1 | ASP | 166 | 25.378 | 30.508 | 59.213 | 1.00 | 13.41 | AAAA |
| ATOM | 1314 | OD2 | ASP | 166 | 27.187 | 29.428 | 58.551 | 1.00 | 16.06 | AAAA |
| ATOM | 1315 | C | ASP | 166 | 25.334 | 30.740 | 62.174 | 1.00 | 15.54 | AAAA |
| ATOM | 1316 | O | ASP | 166 | 24.160 | 30.355 | 62.137 | 1.00 | 12.60 | AAAA |
| ATOM | 1317 | N | LEU | 167 | 25.647 | 32.010 | 62.407 | 1.00 | 14.02 | AAAA |
| ATOM | 1318 | CA | LEU | 167 | 24.598 | 32.993 | 62.665 | 1.00 | 12.05 | AAAA |
| ATOM | 1319 | CB | LEU | 167 | 25.051 | 33.962 | 63.767 | 1.00 | 14.61 | AAAA |
| ATOM | 1320 | CG | LEU | 167 | 25.345 | 33.239 | 65.091 | 1.00 | 17.20 | AAAA |

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Figure 16-21

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1321 | CD1 | LEU | 167 | 25.635 | 34.271 | 66.169 | 1.00 | 28.82 | AAAA |
| ATOM | 1322 | CD2 | LEU | 167 | 24.148 | 32.372 | 65.513 | 1.00 | 18.59 | AAAA |
| ATOM | 1323 | C | LEU | 167 | 24.122 | 33.776 | 61.449 | 1.00 | 12.62 | AAAA |
| ATOM | 1324 | O | LEU | 167 | 23.288 | 34.678 | 61.570 | 1.00 | 15.00 | AAAA |
| ATOM | 1325 | N | ASP | 168 | 24.667 | 33.431 | 60.288 | 1.00 | 14.35 | AAAA |
| ATOM | 1326 | CA | ASP | 168 | 24.277 | 34.056 | 59.022 | 1.00 | 19.50 | AAAA |
| ATOM | 1327 | CB | ASP | 168 | 25.060 | 33.409 | 57.880 | 1.00 | 25.15 | AAAA |
| ATOM | 1328 | CG | ASP | 168 | 24.908 | 34.145 | 56.573 | 1.00 | 48.45 | AAAA |
| ATOM | 1329 | OD1 | ASP | 168 | 25.477 | 35.247 | 56.454 | 1.00 | 64.45 | AAAA |
| ATOM | 1330 | OD2 | ASP | 168 | 24.215 | 33.633 | 55.668 | 1.00 | 44.71 | AAAA |
| ATOM | 1331 | C | ASP | 168 | 22.787 | 33.751 | 58.834 | 1.00 | 16.30 | AAAA |
| ATOM | 1332 | O | ASP | 168 | 22.327 | 32.696 | 59.252 | 1.00 | 17.72 | AAAA |
| ATOM | 1333 | N | ALA | 169 | 22.059 | 34.657 | 58.175 | 1.00 | 14.11 | AAAA |
| ATOM | 1334 | CA | ALA | 169 | 20.618 | 34.503 | 57.934 | 1.00 | 19.61 | AAAA |
| ATOM | 1335 | CB | ALA | 169 | 20.006 | 35.856 | 57.470 | 1.00 | 13.56 | AAAA |
| ATOM | 1336 | C | ALA | 169 | 20.277 | 33.400 | 56.926 | 1.00 | 18.23 | AAAA |
| ATOM | 1337 | O | ALA | 169 | 19.105 | 33.159 | 56.641 | 1.00 | 17.20 | AAAA |
| ATOM | 1338 | N | HIS | 170 | 21.301 | 32.750 | 56.373 | 1.00 | 16.53 | AAAA |
| ATOM | 1339 | CA | HIS | 170 | 21.075 | 31.652 | 55.436 | 1.00 | 17.51 | AAAA |
| ATOM | 1340 | CB | HIS | 170 | 21.616 | 31.973 | 54.033 | 1.00 | 22.32 | AAAA |
| ATOM | 1341 | CG | HIS | 170 | 20.954 | 33.142 | 53.377 | 1.00 | 25.38 | AAAA |
| ATOM | 1342 | CD2 | HIS | 170 | 19.934 | 33.196 | 52.487 | 1.00 | 19.33 | AAAA |
| ATOM | 1343 | ND1 | HIS | 170 | 21.308 | 34.448 | 53.638 | 1.00 | 18.17 | AAAA |
| ATOM | 1344 | CE1 | HIS | 170 | 20.535 | 35.257 | 52.935 | 1.00 | 30.34 | AAAA |
| ATOM | 1345 | NE2 | HIS | 170 | 19.692 | 34.523 | 52.229 | 1.00 | 17.51 | AAAA |
| ATOM | 1346 | C | HIS | 170 | 21.781 | 30.413 | 55.967 | 1.00 | 16.72 | AAAA |
| ATOM | 1347 | O | HIS | 170 | 22.827 | 30.511 | 56.610 | 1.00 | 15.92 | AAAA |
| ATOM | 1348 | N | HIS | 171 | 21.209 | 29.245 | 55.682 | 1.00 | 15.28 | AAAA |
| ATOM | 1349 | CA | HIS | 171 | 21.751 | 27.961 | 56.123 | 1.00 | 12.53 | AAAA |
| ATOM | 1350 | CB | HIS | 171 | 20.702 | 26.878 | 55.814 | 1.00 | 14.09 | AAAA |
| ATOM | 1351 | CG | HIS | 171 | 21.180 | 25.468 | 55.980 | 1.00 | 17.27 | AAAA |
| ATOM | 1352 | CD2 | HIS | 171 | 21.249 | 24.447 | 55.090 | 1.00 | 12.48 | AAAA |
| ATOM | 1353 | ND1 | HIS | 171 | 21.622 | 24.956 | 57.181 | 1.00 | 26.73 | AAAA |
| ATOM | 1354 | CE1 | HIS | 171 | 21.948 | 23.685 | 57.021 | 1.00 | 15.98 | AAAA |
| ATOM | 1355 | NE2 | HIS | 171 | 21.729 | 23.352 | 55.761 | 1.00 | 20.03 | AAAA |
| ATOM | 1356 | C | HIS | 171 | 23.107 | 27.602 | 55.498 | 1.00 | 15.55 | AAAA |
| ATOM | 1357 | O | HIS | 171 | 23.318 | 27.784 | 54.298 | 1.00 | 17.03 | AAAA |
| ATOM | 1358 | N | CYS | 172 | 24.026 | 27.105 | 56.323 | 1.00 | 14.33 | AAAA |
| ATOM | 1359 | CA | CYS | 172 | 25.350 | 26.675 | 55.866 | 1.00 | 13.65 | AAAA |
| ATOM | 1360 | CB | CYS | 172 | 26.330 | 26.631 | 57.054 | 1.00 | 12.99 | AAAA |
| ATOM | 1361 | SG | CYS | 172 | 25.680 | 25.826 | 58.551 | 1.00 | 17.17 | AAAA |
| ATOM | 1362 | C | CYS | 172 | 25.212 | 25.274 | 55.257 | 1.00 | 16.52 | AAAA |
| ATOM | 1363 | O | CYS | 172 | 25.750 | 24.297 | 55.783 | 1.00 | 14.95 | AAAA |
| ATOM | 1364 | N | ASP | 173 | 24.516 | 25.173 | 54.130 | 1.00 | 15.42 | AAAA |
| ATOM | 1365 | CA | ASP | 173 | 24.302 | 23.865 | 53.531 | 1.00 | 14.75 | AAAA |
| ATOM | 1366 | CB | ASP | 173 | 23.339 | 23.956 | 52.332 | 1.00 | 17.73 | AAAA |
| ATOM | 1367 | CG | ASP | 173 | 23.765 | 24.966 | 51.283 | 1.00 | 22.84 | AAAA |
| ATOM | 1368 | OD1 | ASP | 173 | 23.106 | 24.998 | 50.216 | 1.00 | 18.68 | AAAA |
| ATOM | 1369 | OD2 | ASP | 173 | 24.730 | 25.728 | 51.504 | 1.00 | 15.34 | AAAA |
| ATOM | 1370 | C | ASP | 173 | 25.590 | 23.145 | 53.149 | 1.00 | 16.39 | AAAA |
| ATOM | 1371 | O | ASP | 173 | 25.684 | 21.922 | 53.279 | 1.00 | 16.48 | AAAA |
| ATOM | 1372 | N | GLY | 174 | 26.583 | 23.912 | 52.705 | 1.00 | 15.58 | AAAA |
| ATOM | 1373 | CA | GLY | 174 | 27.869 | 23.346 | 52.360 | 1.00 | 13.97 | AAAA |
| ATOM | 1374 | C | GLY | 174 | 28.508 | 22.723 | 53.595 | 1.00 | 18.44 | AAAA |
| ATOM | 1375 | O | GLY | 174 | 28.970 | 21.586 | 53.540 | 1.00 | 15.48 | AAAA |
| ATOM | 1376 | N | VAL | 175 | 28.554 | 23.456 | 54.706 | 1.00 | 16.84 | AAAA |
| ATOM | 1377 | CA | VAL | 175 | 29.136 | 22.923 | 55.946 | 1.00 | 16.54 | AAAA |
| ATOM | 1378 | CB | VAL | 175 | 29.201 | 24.031 | 57.037 | 1.00 | 15.88 | AAAA |
| ATOM | 1379 | CG1 | VAL | 175 | 29.927 | 23.507 | 58.307 | 1.00 | 15.35 | AAAA |
| ATOM | 1380 | CG2 | VAL | 175 | 29.923 | 25.258 | 56.476 | 1.00 | 15.62 | AAAA |
| ATOM | 1381 | C | VAL | 175 | 28.318 | 21.720 | 56.467 | 1.00 | 19.21 | AAAA |
| ATOM | 1382 | O | VAL | 175 | 28.876 | 20.735 | 56.961 | 1.00 | 17.75 | AAAA |
| ATOM | 1383 | N | GLN | 176 | 26.996 | 21.798 | 56.367 | 1.00 | 17.74 | AAAA |
| ATOM | 1384 | CA | GLN | 176 | 26.164 | 20.685 | 56.832 | 1.00 | 15.66 | AAAA |
| ATOM | 1385 | CB | GLN | 176 | 24.678 | 20.973 | 56.595 | 1.00 | 16.64 | AAAA |
| ATOM | 1386 | CG | GLN | 176 | 23.789 | 19.788 | 56.952 | 1.00 | 17.00 | AAAA |

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Figure 16-22

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1387 | CD | GLN | 176 | 22.325 | 20.106 | 56.884 | 1.00 | 21.52 | AAAA |
| ATOM | 1388 | OE1 | GLN | 176 | 21.850 | 21.016 | 57.567 | 1.00 | 21.72 | AAAA |
| ATOM | 1389 | NE2 | GLN | 176 | 21.581 | 19.348 | 56.064 | 1.00 | 20.30 | AAAA |
| ATOM | 1390 | C | GLN | 176 | 26.527 | 19.387 | 56.121 | 1.00 | 16.33 | AAAA |
| ATOM | 1391 | O | GLN | 176 | 26.751 | 18.354 | 56.748 | 1.00 | 17.46 | AAAA |
| ATOM | 1392 | N | GLU | 177 | 26.581 | 19.443 | 54.799 | 1.00 | 22.24 | AAAA |
| ATOM | 1393 | CA | GLU | 177 | 26.909 | 18.251 | 54.021 | 1.00 | 19.67 | AAAA |
| ATOM | 1394 | CB | GLU | 177 | 26.857 | 18.587 | 52.533 | 1.00 | 15.55 | AAAA |
| ATOM | 1395 | CG | GLU | 177 | 27.131 | 17.388 | 51.623 | 1.00 | 20.24 | AAAA |
| ATOM | 1396 | CD | GLU | 177 | 26.960 | 17.740 | 50.159 | 1.00 | 27.00 | AAAA |
| ATOM | 1397 | OE1 | GLU | 177 | 27.974 | 17.935 | 49.450 | 1.00 | 30.23 | AAAA |
| ATOM | 1398 | OE2 | GLU | 177 | 25.796 | 17.853 | 49.725 | 1.00 | 26.89 | AAAA |
| ATOM | 1399 | C | GLU | 177 | 28.284 | 17.713 | 54.376 | 1.00 | 20.42 | AAAA |
| ATOM | 1400 | O | GLU | 177 | 28.486 | 16.503 | 54.527 | 1.00 | 17.05 | AAAA |
| ATOM | 1401 | N | ALA | 178 | 29.233 | 18.626 | 54.527 | 1.00 | 19.67 | AAAA |
| ATOM | 1402 | CA | ALA | 178 | 30.611 | 18.259 | 54.839 | 1.00 | 18.18 | AAAA |
| ATOM | 1403 | CB | ALA | 178 | 31.464 | 19.519 | 54.918 | 1.00 | 12.76 | AAAA |
| ATOM | 1404 | C | ALA | 178 | 30.806 | 17.418 | 56.106 | 1.00 | 17.56 | AAAA |
| ATOM | 1405 | O | ALA | 178 | 31.690 | 16.555 | 56.167 | 1.00 | 17.72 | AAAA |
| ATOM | 1406 | N | PHE | 179 | 29.981 | 17.656 | 57.116 | 1.00 | 18.82 | AAAA |
| ATOM | 1407 | CA | PHE | 179 | 30.124 | 16.945 | 58.379 | 1.00 | 20.26 | AAAA |
| ATOM | 1408 | CB | PHE | 179 | 30.554 | 17.948 | 59.439 | 1.00 | 13.17 | AAAA |
| ATOM | 1409 | CG | PHE | 179 | 31.779 | 18.693 | 59.048 | 1.00 | 16.28 | AAAA |
| ATOM | 1410 | CD1 | PHE | 179 | 31.705 | 20.017 | 58.610 | 1.00 | 13.77 | AAAA |
| ATOM | 1411 | CD2 | PHE | 179 | 33.002 | 18.031 | 58.995 | 1.00 | 15.57 | AAAA |
| ATOM | 1412 | CE1 | PHE | 179 | 32.845 | 20.673 | 58.114 | 1.00 | 20.03 | AAAA |
| ATOM | 1413 | CE2 | PHE | 179 | 34.145 | 18.677 | 58.500 | 1.00 | 20.30 | AAAA |
| ATOM | 1414 | CZ | PHE | 179 | 34.060 | 20.002 | 58.058 | 1.00 | 19.51 | AAAA |
| ATOM | 1415 | C | PHE | 179 | 28.882 | 16.219 | 58.833 | 1.00 | 18.52 | AAAA |
| ATOM | 1416 | O | PHE | 179 | 28.773 | 15.828 | 60.000 | 1.00 | 20.21 | AAAA |
| ATOM | 1417 | N | TYR | 180 | 27.969 | 16.016 | 57.895 | 1.00 | 18.33 | AAAA |
| ATOM | 1418 | CA | TYR | 180 | 26.698 | 15.379 | 58.176 | 1.00 | 19.93 | AAAA |
| ATOM | 1419 | CB | TYR | 180 | 25.874 | 15.310 | 56.894 | 1.00 | 20.97 | AAAA |
| ATOM | 1420 | CG | TYR | 180 | 24.402 | 15.341 | 57.159 | 1.00 | 19.80 | AAAA |
| ATOM | 1421 | CD1 | TYR | 180 | 23.565 | 14.337 | 56.686 | 1.00 | 23.87 | AAAA |
| ATOM | 1422 | CE1 | TYR | 180 | 22.203 | 14.391 | 56.898 | 1.00 | 21.32 | AAAA |
| ATOM | 1423 | CD2 | TYR | 180 | 23.831 | 16.416 | 57.865 | 1.00 | 19.02 | AAAA |
| ATOM | 1424 | CE2 | TYR | 180 | 22.470 | 16.482 | 58.084 | 1.00 | 26.84 | AAAA |
| ATOM | 1425 | CZ | TYR | 180 | 21.659 | 15.462 | 57.594 | 1.00 | 30.54 | AAAA |
| ATOM | 1426 | OH | TYR | 180 | 20.310 | 15.514 | 57.794 | 1.00 | 22.81 | AAAA |
| ATOM | 1427 | C | TYR | 180 | 26.855 | 13.970 | 58.737 | 1.00 | 22.61 | AAAA |
| ATOM | 1428 | O | TYR | 180 | 26.064 | 13.526 | 59.579 | 1.00 | 23.44 | AAAA |
| ATOM | 1429 | N | ASP | 181 | 27.893 | 13.298 | 58.253 | 1.00 | 22.27 | AAAA |
| ATOM | 1430 | CA | ASP | 181 | 28.245 | 11.920 | 58.590 | 1.00 | 33.84 | AAAA |
| ATOM | 1431 | CB | ASP | 181 | 28.916 | 11.318 | 57.339 | 1.00 | 41.74 | AAAA |
| ATOM | 1432 | CG | ASP | 181 | 30.035 | 10.363 | 57.662 | 1.00 | 57.71 | AAAA |
| ATOM | 1433 | OD1 | ASP | 181 | 30.999 | 10.780 | 58.340 | 1.00 | 61.40 | AAAA |
| ATOM | 1434 | OD2 | ASP | 181 | 29.965 | 9.197 | 57.221 | 1.00 | 65.77 | AAAA |
| ATOM | 1435 | C | ASP | 181 | 29.107 | 11.654 | 59.838 | 1.00 | 30.21 | AAAA |
| ATOM | 1436 | O | ASP | 181 | 29.307 | 10.497 | 60.227 | 1.00 | 27.84 | AAAA |
| ATOM | 1437 | N | THR | 182 | 29.615 | 12.696 | 60.480 | 1.00 | 27.53 | AAAA |
| ATOM | 1438 | CA | THR | 182 | 30.472 | 12.466 | 61.634 | 1.00 | 21.19 | AAAA |
| ATOM | 1439 | CB | THR | 182 | 31.918 | 12.977 | 61.358 | 1.00 | 26.55 | AAAA |
| ATOM | 1440 | OG1 | THR | 182 | 32.729 | 12.763 | 62.513 | 1.00 | 25.62 | AAAA |
| ATOM | 1441 | CG2 | THR | 182 | 31.922 | 14.471 | 61.037 | 1.00 | 21.67 | AAAA |
| ATOM | 1442 | C | THR | 182 | 30.010 | 13.050 | 62.954 | 1.00 | 25.02 | AAAA |
| ATOM | 1443 | O | THR | 182 | 29.306 | 14.049 | 62.992 | 1.00 | 23.56 | AAAA |
| ATOM | 1444 | N | ASP | 183 | 30.434 | 12.424 | 64.042 | 1.00 | 19.66 | AAAA |
| ATOM | 1445 | CA | ASP | 183 | 30.086 | 12.894 | 65.371 | 1.00 | 21.52 | AAAA |
| ATOM | 1446 | CB | ASP | 183 | 29.735 | 11.700 | 66.275 | 1.00 | 28.52 | AAAA |
| ATOM | 1447 | CG | ASP | 183 | 30.920 | 10.783 | 66.523 | 1.00 | 32.30 | AAAA |
| ATOM | 1448 | OD1 | ASP | 183 | 31.667 | 10.502 | 65.565 | 1.00 | 30.99 | AAAA |
| ATOM | 1449 | OD2 | ASP | 183 | 31.095 | 10.326 | 67.675 | 1.00 | 48.65 | AAAA |
| ATOM | 1450 | C | ASP | 183 | 31.257 | 13.685 | 65.947 | 1.00 | 16.66 | AAAA |
| ATOM | 1451 | O | ASP | 183 | 31.236 | 14.092 | 67.104 | 1.00 | 23.37 | AAAA |
| ATOM | 1452 | N | GLN | 184 | 32.286 | 13.909 | 65.131 | 1.00 | 21.95 | AAAA |

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Figure 16-23

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1453 | CA | GLN | 184 | 33.437 | 14.672 | 65.590 | 1.00 | 17.65 | AAAA |
| ATOM | 1454 | CB | GLN | 184 | 34.701 | 14.243 | 64.866 | 1.00 | 21.36 | AAAA |
| ATOM | 1455 | CG | GLN | 184 | 35.068 | 12.790 | 65.102 | 1.00 | 27.38 | AAAA |
| ATOM | 1456 | CD | GLN | 184 | 36.485 | 12.476 | 64.691 | 1.00 | 31.96 | AAAA |
| ATOM | 1457 | OE1 | GLN | 184 | 36.899 | 12.760 | 63.573 | 1.00 | 29.90 | AAAA |
| ATOM | 1458 | NE2 | GLN | 184 | 37.239 | 11.878 | 65.599 | 1.00 | 31.84 | AAAA |
| ATOM | 1459 | C | GLN | 184 | 33.207 | 16.165 | 65.382 | 1.00 | 18.54 | AAAA |
| ATOM | 1460 | O | GLN | 184 | 33.881 | 17.009 | 65.972 | 1.00 | 18.11 | AAAA |
| ATOM | 1461 | N | VAL | 185 | 32.258 | 16.481 | 64.519 | 1.00 | 19.18 | AAAA |
| ATOM | 1462 | CA | VAL | 185 | 31.934 | 17.872 | 64.267 | 1.00 | 21.57 | AAAA |
| ATOM | 1463 | CB | VAL | 185 | 32.261 | 18.264 | 62.807 | 1.00 | 22.64 | AAAA |
| ATOM | 1464 | CG1 | VAL | 185 | 31.994 | 19.768 | 62.591 | 1.00 | 16.26 | AAAA |
| ATOM | 1465 | CG2 | VAL | 185 | 33.722 | 17.924 | 62.500 | 1.00 | 16.77 | AAAA |
| ATOM | 1466 | C | VAL | 185 | 30.449 | 18.035 | 64.523 | 1.00 | 15.91 | AAAA |
| ATOM | 1467 | O | VAL | 185 | 29.658 | 17.156 | 64.179 | 1.00 | 20.79 | AAAA |
| ATOM | 1468 | N | PHE | 186 | 30.081 | 19.146 | 65.153 | 1.00 | 18.73 | AAAA |
| ATOM | 1469 | CA | PHE | 186 | 28.687 | 19.446 | 65.435 | 1.00 | 16.22 | AAAA |
| ATOM | 1470 | CB | PHE | 186 | 28.432 | 19.559 | 66.952 | 1.00 | 16.83 | AAAA |
| ATOM | 1471 | CG | PHE | 186 | 26.976 | 19.682 | 67.299 | 1.00 | 17.96 | AAAA |
| ATOM | 1472 | CD1 | PHE | 186 | 26.319 | 18.656 | 67.968 | 1.00 | 23.24 | AAAA |
| ATOM | 1473 | CD2 | PHE | 186 | 26.240 | 20.797 | 66.904 | 1.00 | 15.41 | AAAA |
| ATOM | 1474 | CE1 | PHE | 186 | 24.953 | 18.738 | 68.235 | 1.00 | 18.99 | AAAA |
| ATOM | 1475 | CE2 | PHE | 186 | 24.879 | 20.887 | 67.168 | 1.00 | 24.05 | AAAA |
| ATOM | 1476 | CZ | PHE | 186 | 24.234 | 19.846 | 67.838 | 1.00 | 22.93 | AAAA |
| ATOM | 1477 | C | PHE | 186 | 28.437 | 20.789 | 64.778 | 1.00 | 17.16 | AAAA |
| ATOM | 1478 | O | PHE | 186 | 29.192 | 21.725 | 64.993 | 1.00 | 19.37 | AAAA |
| ATOM | 1479 | N | VAL | 187 | 27.391 | 20.874 | 63.961 | 1.00 | 19.67 | AAAA |
| ATOM | 1480 | CA | VAL | 187 | 27.075 | 22.116 | 63.277 | 1.00 | 17.74 | AAAA |
| ATOM | 1481 | CB | VAL | 187 | 27.010 | 21.914 | 61.720 | 1.00 | 18.65 | AAAA |
| ATOM | 1482 | CG1 | VAL | 187 | 26.578 | 23.211 | 61.024 | 1.00 | 17.31 | AAAA |
| ATOM | 1483 | CG2 | VAL | 187 | 28.359 | 21.453 | 61.194 | 1.00 | 16.65 | AAAA |
| ATOM | 1484 | C | VAL | 187 | 25.732 | 22.637 | 63.746 | 1.00 | 18.46 | AAAA |
| ATOM | 1485 | O | VAL | 187 | 24.752 | 21.903 | 63.764 | 1.00 | 20.64 | AAAA |
| ATOM | 1486 | N | LEU | 188 | 25.708 | 23.899 | 64.150 | 1.00 | 14.42 | AAAA |
| ATOM | 1487 | CA | LEU | 188 | 24.482 | 24.563 | 64.567 | 1.00 | 16.68 | AAAA |
| ATOM | 1488 | CB | LEU | 188 | 24.568 | 25.070 | 66.009 | 1.00 | 13.98 | AAAA |
| ATOM | 1489 | CG | LEU | 188 | 23.522 | 26.119 | 66.450 | 1.00 | 13.66 | AAAA |
| ATOM | 1490 | CD1 | LEU | 188 | 22.103 | 25.556 | 66.401 | 1.00 | 15.55 | AAAA |
| ATOM | 1491 | CD2 | LEU | 188 | 23.844 | 26.585 | 67.861 | 1.00 | 16.40 | AAAA |
| ATOM | 1492 | C | LEU | 188 | 24.272 | 25.756 | 63.667 | 1.00 | 20.01 | AAAA |
| ATOM | 1493 | O | LEU | 188 | 25.164 | 26.595 | 63.506 | 1.00 | 18.86 | AAAA |
| ATOM | 1494 | N | SER | 189 | 23.106 | 25.845 | 63.057 | 1.00 | 14.46 | AAAA |
| ATOM | 1495 | CA | SER | 189 | 22.841 | 27.011 | 62.230 | 1.00 | 14.56 | AAAA |
| ATOM | 1496 | CB | SER | 189 | 22.896 | 26.668 | 60.737 | 1.00 | 15.55 | AAAA |
| ATOM | 1497 | OG | SER | 189 | 22.619 | 27.851 | 60.008 | 1.00 | 14.09 | AAAA |
| ATOM | 1498 | C | SER | 189 | 21.487 | 27.606 | 62.508 | 1.00 | 15.24 | AAAA |
| ATOM | 1499 | O | SER | 189 | 20.509 | 26.885 | 62.578 | 1.00 | 21.46 | AAAA |
| ATOM | 1500 | N | LEU | 190 | 21.423 | 28.921 | 62.690 | 1.00 | 14.92 | AAAA |
| ATOM | 1501 | CA | LEU | 190 | 20.128 | 29.572 | 62.826 | 1.00 | 15.54 | AAAA |
| ATOM | 1502 | CB | LEU | 190 | 20.084 | 30.663 | 63.906 | 1.00 | 21.02 | AAAA |
| ATOM | 1503 | CG | LEU | 190 | 20.594 | 30.532 | 65.339 | 1.00 | 30.17 | AAAA |
| ATOM | 1504 | CD1 | LEU | 190 | 19.736 | 31.437 | 66.210 | 1.00 | 19.75 | AAAA |
| ATOM | 1505 | CD2 | LEU | 190 | 20.547 | 29.130 | 65.831 | 1.00 | 19.08 | AAAA |
| ATOM | 1506 | C | LEU | 190 | 20.035 | 30.250 | 61.456 | 1.00 | 14.31 | AAAA |
| ATOM | 1507 | O | LEU | 190 | 21.031 | 30.752 | 60.951 | 1.00 | 15.43 | AAAA |
| ATOM | 1508 | N | HIS | 191 | 18.855 | 30.285 | 60.856 | 1.00 | 16.88 | AAAA |
| ATOM | 1509 | CA | HIS | 191 | 18.732 | 30.884 | 59.535 | 1.00 | 14.34 | AAAA |
| ATOM | 1510 | CB | HIS | 191 | 19.506 | 30.015 | 58.539 | 1.00 | 17.34 | AAAA |
| ATOM | 1511 | CG | HIS | 191 | 19.229 | 28.546 | 58.697 | 1.00 | 14.27 | AAAA |
| ATOM | 1512 | CD2 | HIS | 191 | 19.941 | 27.578 | 59.319 | 1.00 | 9.60 | AAAA |
| ATOM | 1513 | ND1 | HIS | 191 | 18.073 | 27.940 | 58.247 | 1.00 | 21.22 | AAAA |
| ATOM | 1514 | CE1 | HIS | 191 | 18.088 | 26.660 | 58.582 | 1.00 | 17.22 | AAAA |
| ATOM | 1515 | NE2 | HIS | 191 | 19.212 | 26.415 | 59.232 | 1.00 | 20.70 | AAAA |
| ATOM | 1516 | C | HIS | 191 | 17.277 | 31.026 | 59.110 | 1.00 | 16.19 | AAAA |
| ATOM | 1517 | O | HIS | 191 | 16.381 | 30.489 | 59.766 | 1.00 | 16.73 | AAAA |
| ATOM | 1518 | N | GLN | 192 | 17.044 | 31.796 | 58.045 | 1.00 | 14.78 | AAAA |

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Figure 16-24

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1519 | CA | GLN | 192 | 15.683 | 31.968 | 57.516 | 1.00 | 16.33 | AAAA |
| ATOM | 1520 | CB | GLN | 192 | 15.669 | 32.871 | 56.283 | 1.00 | 17.07 | AAAA |
| ATOM | 1521 | CG | GLN | 192 | 16.174 | 34.270 | 56.498 | 1.00 | 18.15 | AAAA |
| ATOM | 1522 | CD | GLN | 192 | 16.408 | 34.965 | 55.177 | 1.00 | 14.74 | AAAA |
| ATOM | 1523 | OE1 | GLN | 192 | 15.490 | 35.566 | 54.587 | 1.00 | 20.46 | AAAA |
| ATOM | 1524 | NE2 | GLN | 192 | 17.630 | 34.839 | 54.665 | 1.00 | 13.44 | AAAA |
| ATOM | 1525 | C | GLN | 192 | 15.262 | 30.584 | 57.072 | 1.00 | 15.06 | AAAA |
| ATOM | 1526 | O | GLN | 192 | 16.071 | 29.843 | 56.514 | 1.00 | 19.23 | AAAA |
| ATOM | 1527 | N | SER | 193 | 14.007 | 30.223 | 57.304 | 1.00 | 15.63 | AAAA |
| ATOM | 1528 | CA | SER | 193 | 13.561 | 28.907 | 56.877 | 1.00 | 13.84 | AAAA |
| ATOM | 1529 | CB | SER | 193 | 12.097 | 28.677 | 57.284 | 1.00 | 17.28 | AAAA |
| ATOM | 1530 | OG | SER | 193 | 11.639 | 27.439 | 56.750 | 1.00 | 17.58 | AAAA |
| ATOM | 1531 | C | SER | 193 | 13.687 | 28.704 | 55.350 | 1.00 | 11.80 | AAAA |
| ATOM | 1532 | O | SER | 193 | 13.400 | 29.601 | 54.569 | 1.00 | 18.44 | AAAA |
| ATOM | 1533 | N | PRO | 194 | 14.103 | 27.505 | 54.928 | 1.00 | 14.59 | AAAA |
| ATOM | 1534 | CD | PRO | 194 | 14.335 | 26.325 | 55.782 | 1.00 | 19.22 | AAAA |
| ATOM | 1535 | CA | PRO | 194 | 14.268 | 27.143 | 53.513 | 1.00 | 15.30 | AAAA |
| ATOM | 1536 | CB | PRO | 194 | 14.892 | 25.737 | 53.573 | 1.00 | 18.33 | AAAA |
| ATOM | 1537 | CG | PRO | 194 | 15.359 | 25.587 | 55.007 | 1.00 | 22.34 | AAAA |
| ATOM | 1538 | C | PRO | 194 | 12.880 | 27.104 | 52.866 | 1.00 | 16.40 | AAAA |
| ATOM | 1539 | O | PRO | 194 | 12.757 | 27.003 | 51.640 | 1.00 | 19.43 | AAAA |
| ATOM | 1540 | N | GLU | 195 | 11.828 | 27.151 | 53.681 | 1.00 | 20.57 | AAAA |
| ATOM | 1541 | CA | GLU | 195 | 10.483 | 27.161 | 53.099 | 1.00 | 30.15 | AAAA |
| ATOM | 1542 | CB | GLU | 195 | 9.386 | 27.037 | 54.173 | 1.00 | 31.91 | AAAA |
| ATOM | 1543 | CG | GLU | 195 | 8.987 | 28.325 | 54.879 | 1.00 | 45.60 | AAAA |
| ATOM | 1544 | CD | GLU | 195 | 7.880 | 29.119 | 54.174 | 1.00 | 34.45 | AAAA |
| ATOM | 1545 | OE1 | GLU | 195 | 7.635 | 30.259 | 54.612 | 1.00 | 43.98 | AAAA |
| ATOM | 1546 | OE2 | GLU | 195 | 7.241 | 28.627 | 53.210 | 1.00 | 38.39 | AAAA |
| ATOM | 1547 | C | GLU | 195 | 10.333 | 28.474 | 52.318 | 1.00 | 26.92 | AAAA |
| ATOM | 1548 | O | GLU | 195 | 9.522 | 28.557 | 51.395 | 1.00 | 24.59 | AAAA |
| ATOM | 1549 | N | TYR | 196 | 11.116 | 29.501 | 52.669 | 1.00 | 18.16 | AAAA |
| ATOM | 1550 | CA | TYR | 196 | 11.024 | 30.753 | 51.922 | 1.00 | 15.81 | AAAA |
| ATOM | 1551 | CB | TYR | 196 | 10.208 | 31.801 | 52.690 | 1.00 | 20.01 | AAAA |
| ATOM | 1552 | CG | TYR | 196 | 10.868 | 32.353 | 53.932 | 1.00 | 19.77 | AAAA |
| ATOM | 1553 | CD1 | TYR | 196 | 11.779 | 33.408 | 53.853 | 1.00 | 18.24 | AAAA |
| ATOM | 1554 | CE1 | TYR | 196 | 12.407 | 33.898 | 54.988 | 1.00 | 18.50 | AAAA |
| ATOM | 1555 | CD2 | TYR | 196 | 10.598 | 31.801 | 55.185 | 1.00 | 18.12 | AAAA |
| ATOM | 1556 | CE2 | TYR | 196 | 11.223 | 32.283 | 56.339 | 1.00 | 21.09 | AAAA |
| ATOM | 1557 | CZ | TYR | 196 | 12.125 | 33.326 | 56.235 | 1.00 | 20.39 | AAAA |
| ATOM | 1558 | OH | TYR | 196 | 12.759 | 33.784 | 57.367 | 1.00 | 16.20 | AAAA |
| ATOM | 1559 | C | TYR | 196 | 12.342 | 31.372 | 51.475 | 1.00 | 16.89 | AAAA |
| ATOM | 1560 | O | TYR | 196 | 12.336 | 32.347 | 50.718 | 1.00 | 23.08 | AAAA |
| ATOM | 1561 | N | ALA | 197 | 13.466 | 30.817 | 51.911 | 1.00 | 17.52 | AAAA |
| ATOM | 1562 | CA | ALA | 197 | 14.754 | 31.400 | 51.512 | 1.00 | 20.26 | AAAA |
| ATOM | 1563 | CB | ALA | 197 | 15.315 | 32.261 | 52.659 | 1.00 | 20.74 | AAAA |
| ATOM | 1564 | C | ALA | 197 | 15.814 | 30.392 | 51.074 | 1.00 | 13.51 | AAAA |
| ATOM | 1565 | O | ALA | 197 | 15.787 | 29.229 | 51.457 | 1.00 | 19.35 | AAAA |
| ATOM | 1566 | N | PHE | 198 | 16.757 | 30.869 | 50.257 | 1.00 | 18.01 | AAAA |
| ATOM | 1567 | CA | PHE | 198 | 17.861 | 30.049 | 49.782 | 1.00 | 17.97 | AAAA |
| ATOM | 1568 | CB | PHE | 198 | 18.929 | 30.933 | 49.119 | 1.00 | 20.38 | AAAA |
| ATOM | 1569 | CG | PHE | 198 | 20.094 | 30.162 | 48.545 | 1.00 | 23.61 | AAAA |
| ATOM | 1570 | CD1 | PHE | 198 | 20.039 | 29.660 | 47.245 | 1.00 | 29.71 | AAAA |
| ATOM | 1571 | CD2 | PHE | 198 | 21.229 | 29.899 | 49.321 | 1.00 | 19.06 | AAAA |
| ATOM | 1572 | CE1 | PHE | 198 | 21.091 | 28.908 | 46.719 | 1.00 | 30.39 | AAAA |
| ATOM | 1573 | CE2 | PHE | 198 | 22.290 | 29.145 | 48.807 | 1.00 | 23.17 | AAAA |
| ATOM | 1574 | CZ | PHE | 198 | 22.218 | 28.646 | 47.493 | 1.00 | 22.74 | AAAA |
| ATOM | 1575 | C | PHE | 198 | 18.453 | 29.419 | 51.032 | 1.00 | 16.02 | AAAA |
| ATOM | 1576 | O | PHE | 198 | 18.552 | 30.073 | 52.061 | 1.00 | 20.95 | AAAA |
| ATOM | 1577 | N | PRO | 199 | 18.941 | 28.176 | 50.937 | 1.00 | 19.92 | AAAA |
| ATOM | 1578 | CD | PRO | 199 | 19.600 | 27.508 | 52.074 | 1.00 | 17.86 | AAAA |
| ATOM | 1579 | CA | PRO | 199 | 18.990 | 27.318 | 49.744 | 1.00 | 23.54 | AAAA |
| ATOM | 1580 | CB | PRO | 199 | 20.108 | 26.344 | 50.095 | 1.00 | 22.70 | AAAA |
| ATOM | 1581 | CG | PRO | 199 | 19.813 | 26.087 | 51.534 | 1.00 | 23.16 | AAAA |
| ATOM | 1582 | C | PRO | 199 | 17.710 | 26.595 | 49.312 | 1.00 | 30.97 | AAAA |
| ATOM | 1583 | O | PRO | 199 | 17.733 | 25.855 | 48.322 | 1.00 | 23.25 | AAAA |
| ATOM | 1584 | N | PHE | 200 | 16.621 | 26.795 | 50.054 | 1.00 | 20.32 | AAAA |

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Figure 16-25

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1585 | CA | PHE | 200 | 15.319 | 26.166 | 49.752 | 1.00 | 20.27 | AAAA |
| ATOM | 1586 | CB | PHE | 200 | 14.840 | 26.533 | 48.346 | 1.00 | 19.77 | AAAA |
| ATOM | 1587 | CG | PHE | 200 | 14.752 | 27.999 | 48.082 | 1.00 | 18.06 | AAAA |
| ATOM | 1588 | CD1 | PHE | 200 | 15.742 | 28.644 | 47.346 | 1.00 | 18.97 | AAAA |
| ATOM | 1589 | CD2 | PHE | 200 | 13.654 | 28.736 | 48.519 | 1.00 | 19.06 | AAAA |
| ATOM | 1590 | CE1 | PHE | 200 | 15.635 | 30.003 | 47.042 | 1.00 | 21.67 | AAAA |
| ATOM | 1591 | CE2 | PHE | 200 | 13.539 | 30.101 | 48.221 | 1.00 | 22.60 | AAAA |
| ATOM | 1592 | CZ | PHE | 200 | 14.527 | 30.736 | 47.482 | 1.00 | 18.93 | AAAA |
| ATOM | 1593 | C | PHE | 200 | 15.294 | 24.637 | 49.845 | 1.00 | 18.44 | AAAA |
| ATOM | 1594 | O | PHE | 200 | 14.302 | 24.049 | 50.272 | 1.00 | 20.74 | AAAA |
| ATOM | 1595 | N | GLU | 201 | 16.384 | 24.004 | 49.418 | 1.00 | 20.77 | AAAA |
| ATOM | 1596 | CA | GLU | 201 | 16.522 | 22.542 | 49.399 | 1.00 | 27.34 | AAAA |
| ATOM | 1597 | CB | GLU | 201 | 17.498 | 22.146 | 48.284 | 1.00 | 28.99 | AAAA |
| ATOM | 1598 | CG | GLU | 201 | 17.024 | 22.458 | 46.881 | 1.00 | 34.82 | AAAA |
| ATOM | 1599 | CD | GLU | 201 | 18.123 | 22.265 | 45.848 | 1.00 | 32.40 | AAAA |
| ATOM | 1600 | OE1 | GLU | 201 | 18.701 | 21.155 | 45.769 | 1.00 | 38.28 | AAAA |
| ATOM | 1601 | OE2 | GLU | 201 | 18.405 | 23.230 | 45.111 | 1.00 | 40.08 | AAAA |
| ATOM | 1602 | C | GLU | 201 | 17.007 | 21.891 | 50.695 | 1.00 | 23.51 | AAAA |
| ATOM | 1603 | O | GLU | 201 | 16.845 | 20.689 | 50.886 | 1.00 | 23.17 | AAAA |
| ATOM | 1604 | N | LYS | 202 | 17.619 | 22.681 | 51.571 | 1.00 | 20.03 | AAAA |
| ATOM | 1605 | CA | LYS | 202 | 18.178 | 22.177 | 52.829 | 1.00 | 17.01 | AAAA |
| ATOM | 1606 | CB | LYS | 202 | 19.666 | 21.862 | 52.634 | 1.00 | 19.24 | AAAA |
| ATOM | 1607 | CG | LYS | 202 | 19.903 | 20.769 | 51.611 | 1.00 | 36.04 | AAAA |
| ATOM | 1608 | CD | LYS | 202 | 20.997 | 21.162 | 50.648 | 1.00 | 45.11 | AAAA |
| ATOM | 1609 | CE | LYS | 202 | 21.060 | 20.209 | 49.463 | 1.00 | 55.83 | AAAA |
| ATOM | 1610 | NZ | LYS | 202 | 22.024 | 20.662 | 48.422 | 1.00 | 28.09 | AAAA |
| ATOM | 1611 | C | LYS | 202 | 18.016 | 23.240 | 53.899 | 1.00 | 17.02 | AAAA |
| ATOM | 1612 | O | LYS | 202 | 17.705 | 24.381 | 53.585 | 1.00 | 20.20 | AAAA |
| ATOM | 1613 | N | GLY | 203 | 18.232 | 22.875 | 55.160 | 1.00 | 22.94 | AAAA |
| ATOM | 1614 | CA | GLY | 203 | 18.064 | 23.850 | 56.223 | 1.00 | 19.38 | AAAA |
| ATOM | 1615 | C | GLY | 203 | 16.874 | 23.564 | 57.128 | 1.00 | 20.48 | AAAA |
| ATOM | 1616 | O | GLY | 203 | 16.607 | 24.312 | 58.070 | 1.00 | 18.55 | AAAA |
| ATOM | 1617 | N | PHE | 204 | 16.150 | 22.484 | 56.852 | 1.00 | 15.42 | AAAA |
| ATOM | 1618 | CA | PHE | 204 | 14.983 | 22.143 | 57.670 | 1.00 | 20.73 | AAAA |
| ATOM | 1619 | CB | PHE | 204 | 14.018 | 21.212 | 56.903 | 1.00 | 19.97 | AAAA |
| ATOM | 1620 | CG | PHE | 204 | 13.441 | 21.838 | 55.667 | 1.00 | 19.63 | AAAA |
| ATOM | 1621 | CD1 | PHE | 204 | 14.137 | 21.801 | 54.459 | 1.00 | 24.96 | AAAA |
| ATOM | 1622 | CD2 | PHE | 204 | 12.230 | 22.523 | 55.725 | 1.00 | 18.92 | AAAA |
| ATOM | 1623 | CE1 | PHE | 204 | 13.636 | 22.438 | 53.327 | 1.00 | 20.66 | AAAA |
| ATOM | 1624 | CE2 | PHE | 204 | 11.720 | 23.169 | 54.597 | 1.00 | 24.86 | AAAA |
| ATOM | 1625 | CZ | PHE | 204 | 12.422 | 23.127 | 53.400 | 1.00 | 23.66 | AAAA |
| ATOM | 1626 | C | PHE | 204 | 15.376 | 21.513 | 59.006 | 1.00 | 18.73 | AAAA |
| ATOM | 1627 | O | PHE | 204 | 16.415 | 20.851 | 59.131 | 1.00 | 20.18 | AAAA |
| ATOM | 1628 | N | LEU | 205 | 14.518 | 21.726 | 59.994 | 1.00 | 19.46 | AAAA |
| ATOM | 1629 | CA | LEU | 205 | 14.727 | 21.244 | 61.356 | 1.00 | 21.09 | AAAA |
| ATOM | 1630 | CB | LEU | 205 | 13.547 | 21.674 | 62.233 | 1.00 | 23.44 | AAAA |
| ATOM | 1631 | CG | LEU | 205 | 13.506 | 21.222 | 63.693 | 1.00 | 23.23 | AAAA |
| ATOM | 1632 | CD1 | LEU | 205 | 14.717 | 21.736 | 64.445 | 1.00 | 24.06 | AAAA |
| ATOM | 1633 | CD2 | LEU | 205 | 12.224 | 21.743 | 64.312 | 1.00 | 30.63 | AAAA |
| ATOM | 1634 | C | LEU | 205 | 14.943 | 19.748 | 61.489 | 1.00 | 23.53 | AAAA |
| ATOM | 1635 | O | LEU | 205 | 15.659 | 19.315 | 62.381 | 1.00 | 21.28 | AAAA |
| ATOM | 1636 | N | GLU | 206 | 14.356 | 18.959 | 60.591 | 1.00 | 21.59 | AAAA |
| ATOM | 1637 | CA | GLU | 206 | 14.487 | 17.502 | 60.686 | 1.00 | 27.89 | AAAA |
| ATOM | 1638 | CB | GLU | 206 | 13.345 | 16.816 | 59.928 | 1.00 | 28.90 | AAAA |
| ATOM | 1639 | CG | GLU | 206 | 12.060 | 17.615 | 59.942 | 1.00 | 48.55 | AAAA |
| ATOM | 1640 | CD | GLU | 206 | 12.169 | 18.832 | 59.042 | 1.00 | 46.86 | AAAA |
| ATOM | 1641 | OE1 | GLU | 206 | 11.360 | 19.769 | 59.178 | 1.00 | 21.58 | AAAA |
| ATOM | 1642 | OE2 | GLU | 206 | 13.076 | 18.833 | 58.181 | 1.00 | 63.58 | AAAA |
| ATOM | 1643 | C | GLU | 206 | 15.819 | 16.955 | 60.188 | 1.00 | 22.86 | AAAA |
| ATOM | 1644 | O | GLU | 206 | 16.071 | 15.753 | 60.286 | 1.00 | 21.21 | AAAA |
| ATOM | 1645 | N | GLU | 207 | 16.666 | 17.816 | 59.631 | 1.00 | 25.04 | AAAA |
| ATOM | 1646 | CA | GLU | 207 | 17.976 | 17.373 | 59.152 | 1.00 | 19.61 | AAAA |
| ATOM | 1647 | CB | GLU | 207 | 18.483 | 18.322 | 58.055 | 1.00 | 20.75 | AAAA |
| ATOM | 1648 | CG | GLU | 207 | 17.682 | 18.222 | 56.753 | 1.00 | 18.44 | AAAA |
| ATOM | 1649 | CD | GLU | 207 | 17.687 | 19.514 | 55.983 | 1.00 | 24.75 | AAAA |
| ATOM | 1650 | OE1 | GLU | 207 | 18.738 | 20.182 | 55.948 | 1.00 | 22.17 | AAAA |

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Figure 16-26

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1651 | OE2 | GLU | 207 | 16.646 | 19.854 | 55.396 | 1.00 | 15.50 | AAAA |
| ATOM | 1652 | C | GLU | 207 | 18.921 | 17.379 | 60.350 | 1.00 | 28.83 | AAAA |
| ATOM | 1653 | O | GLU | 207 | 19.506 | 18.416 | 60.687 | 1.00 | 18.11 | AAAA |
| ATOM | 1654 | N | ILE | 208 | 19.081 | 16.218 | 60.988 | 1.00 | 21.60 | AAAA |
| ATOM | 1655 | CA | ILE | 208 | 19.930 | 16.138 | 62.168 | 1.00 | 22.37 | AAAA |
| ATOM | 1656 | CB | ILE | 208 | 19.113 | 15.652 | 63.403 | 1.00 | 28.84 | AAAA |
| ATOM | 1657 | CG2 | ILE | 208 | 19.968 | 15.693 | 64.653 | 1.00 | 43.26 | AAAA |
| ATOM | 1658 | CG1 | ILE | 208 | 17.905 | 16.561 | 63.625 | 1.00 | 21.61 | AAAA |
| ATOM | 1659 | CD1 | ILE | 208 | 17.029 | 16.160 | 64.786 | 1.00 | 41.40 | AAAA |
| ATOM | 1660 | C | ILE | 208 | 21.156 | 15.260 | 61.981 | 1.00 | 24.74 | AAAA |
| ATOM | 1661 | O | ILE | 208 | 21.785 | 14.850 | 62.943 | 1.00 | 22.68 | AAAA |
| ATOM | 1662 | N | GLY | 209 | 21.512 | 14.969 | 60.738 | 1.00 | 22.80 | AAAA |
| ATOM | 1663 | CA | GLY | 209 | 22.690 | 14.153 | 60.535 | 1.00 | 20.43 | AAAA |
| ATOM | 1664 | C | GLY | 209 | 22.342 | 12.769 | 60.037 | 1.00 | 25.56 | AAAA |
| ATOM | 1665 | O | GLY | 209 | 21.165 | 12.447 | 59.850 | 1.00 | 25.22 | AAAA |
| ATOM | 1666 | N | GLU | 210 | 23.373 | 11.944 | 59.888 | 1.00 | 26.07 | AAAA |
| ATOM | 1667 | CA | GLU | 210 | 23.235 | 10.601 | 59.348 | 1.00 | 25.78 | AAAA |
| ATOM | 1668 | CB | GLU | 210 | 23.404 | 10.731 | 57.835 | 1.00 | 28.27 | AAAA |
| ATOM | 1669 | CG | GLU | 210 | 23.041 | 9.569 | 56.965 | 1.00 | 56.41 | AAAA |
| ATOM | 1670 | CD | GLU | 210 | 23.170 | 9.952 | 55.495 | 1.00 | 65.37 | AAAA |
| ATOM | 1671 | OE1 | GLU | 210 | 24.290 | 10.327 | 55.075 | 1.00 | 62.00 | AAAA |
| ATOM | 1672 | OE2 | GLU | 210 | 22.153 | 9.894 | 54.768 | 1.00 | 73.24 | AAAA |
| ATOM | 1673 | C | GLU | 210 | 24.329 | 9.709 | 59.936 | 1.00 | 31.85 | AAAA |
| ATOM | 1674 | O | GLU | 210 | 25.447 | 10.170 | 60.217 | 1.00 | 28.85 | AAAA |
| ATOM | 1675 | N | GLY | 211 | 24.012 | 8.431 | 60.121 | 1.00 | 27.84 | AAAA |
| ATOM | 1676 | CA | GLY | 211 | 24.991 | 7.502 | 60.657 | 1.00 | 26.25 | AAAA |
| ATOM | 1677 | C | GLY | 211 | 25.545 | 7.942 | 61.995 | 1.00 | 27.79 | AAAA |
| ATOM | 1678 | O | GLY | 211 | 24.788 | 8.324 | 62.874 | 1.00 | 28.66 | AAAA |
| ATOM | 1679 | N | LYS | 212 | 26.865 | 7.880 | 62.150 | 1.00 | 34.62 | AAAA |
| ATOM | 1680 | CA | LYS | 212 | 27.512 | 8.287 | 63.393 | 1.00 | 34.39 | AAAA |
| ATOM | 1681 | CB | LYS | 212 | 29.029 | 8.132 | 63.273 | 1.00 | 40.40 | AAAA |
| ATOM | 1682 | CG | LYS | 212 | 29.505 | 6.712 | 62.996 | 1.00 | 53.97 | AAAA |
| ATOM | 1683 | CD | LYS | 212 | 29.139 | 5.770 | 64.131 | 1.00 | 61.93 | AAAA |
| ATOM | 1684 | CE | LYS | 212 | 29.612 | 4.347 | 63.863 | 1.00 | 62.74 | AAAA |
| ATOM | 1685 | NZ | LYS | 212 | 31.091 | 4.256 | 63.711 | 1.00 | 70.11 | AAAA |
| ATOM | 1686 | C | LYS | 212 | 27.181 | 9.741 | 63.725 | 1.00 | 36.04 | AAAA |
| ATOM | 1687 | O | LYS | 212 | 27.109 | 10.126 | 64.897 | 1.00 | 28.34 | AAAA |
| ATOM | 1688 | N | GLY | 213 | 26.959 | 10.543 | 62.688 | 1.00 | 31.47 | AAAA |
| ATOM | 1689 | CA | GLY | 213 | 26.648 | 11.948 | 62.898 | 1.00 | 31.68 | AAAA |
| ATOM | 1690 | C | GLY | 213 | 25.189 | 12.291 | 63.142 | 1.00 | 28.78 | AAAA |
| ATOM | 1691 | O | GLY | 213 | 24.840 | 13.460 | 63.259 | 1.00 | 22.56 | AAAA |
| ATOM | 1692 | N | LYS | 214 | 24.317 | 11.292 | 63.222 | 1.00 | 28.54 | AAAA |
| ATOM | 1693 | CA | LYS | 214 | 22.905 | 11.585 | 63.463 | 1.00 | 31.11 | AAAA |
| ATOM | 1694 | CB | LYS | 214 | 22.080 | 10.295 | 63.325 | 1.00 | 31.03 | AAAA |
| ATOM | 1695 | CG | LYS | 214 | 20.583 | 10.461 | 63.224 | 1.00 | 38.15 | AAAA |
| ATOM | 1696 | CD | LYS | 214 | 19.968 | 9.115 | 62.844 | 1.00 | 40.49 | AAAA |
| ATOM | 1697 | CE | LYS | 214 | 18.490 | 9.220 | 62.537 | 1.00 | 48.02 | AAAA |
| ATOM | 1698 | NZ | LYS | 214 | 17.927 | 7.924 | 62.064 | 1.00 | 44.99 | AAAA |
| ATOM | 1699 | C | LYS | 214 | 22.834 | 12.160 | 64.875 | 1.00 | 26.90 | AAAA |
| ATOM | 1700 | O | LYS | 214 | 23.260 | 11.524 | 65.831 | 1.00 | 33.33 | AAAA |
| ATOM | 1701 | N | GLY | 215 | 22.310 | 13.376 | 64.997 | 1.00 | 24.38 | AAAA |
| ATOM | 1702 | CA | GLY | 215 | 22.230 | 14.034 | 66.290 | 1.00 | 26.03 | AAAA |
| ATOM | 1703 | C | GLY | 215 | 23.298 | 15.115 | 66.447 | 1.00 | 27.03 | AAAA |
| ATOM | 1704 | O | GLY | 215 | 23.352 | 15.820 | 67.458 | 1.00 | 23.34 | AAAA |
| ATOM | 1705 | N | TYR | 216 | 24.152 | 15.260 | 65.439 | 1.00 | 22.79 | AAAA |
| ATOM | 1706 | CA | TYR | 216 | 25.217 | 16.257 | 65.512 | 1.00 | 25.51 | AAAA |
| ATOM | 1707 | CB | TYR | 216 | 26.592 | 15.576 | 65.406 | 1.00 | 20.54 | AAAA |
| ATOM | 1708 | CG | TYR | 216 | 26.900 | 14.671 | 66.581 | 1.00 | 26.47 | AAAA |
| ATOM | 1709 | CD1 | TYR | 216 | 26.221 | 13.464 | 66.757 | 1.00 | 28.96 | AAAA |
| ATOM | 1710 | CE1 | TYR | 216 | 26.455 | 12.660 | 67.872 | 1.00 | 33.08 | AAAA |
| ATOM | 1711 | CD2 | TYR | 216 | 27.832 | 15.052 | 67.552 | 1.00 | 24.21 | AAAA |
| ATOM | 1712 | CE2 | TYR | 216 | 28.074 | 14.254 | 68.675 | 1.00 | 34.45 | AAAA |
| ATOM | 1713 | CZ | TYR | 216 | 27.378 | 13.063 | 68.827 | 1.00 | 40.53 | AAAA |
| ATOM | 1714 | OH | TYR | 216 | 27.580 | 12.291 | 69.947 | 1.00 | 45.67 | AAAA |
| ATOM | 1715 | C | TYR | 216 | 25.104 | 17.391 | 64.493 | 1.00 | 22.57 | AAAA |
| ATOM | 1716 | O | TYR | 216 | 26.097 | 18.014 | 64.126 | 1.00 | 19.70 | AAAA |

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Figure 16-27

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1717 | N | ASN | 217 | 23.889 | 17.635 | 64.027 | 1.00 | 22.88 | AAAA |
| ATOM | 1718 | CA | ASN | 217 | 23.621 | 18.729 | 63.109 | 1.00 | 22.60 | AAAA |
| ATOM | 1719 | CB | ASN | 217 | 23.453 | 18.240 | 61.671 | 1.00 | 16.61 | AAAA |
| ATOM | 1720 | CG | ASN | 217 | 23.233 | 19.387 | 60.695 | 1.00 | 17.16 | AAAA |
| ATOM | 1721 | OD1 | ASN | 217 | 22.098 | 19.704 | 60.307 | 1.00 | 20.23 | AAAA |
| ATOM | 1722 | ND2 | ASN | 217 | 24.320 | 20.032 | 60.309 | 1.00 | 12.18 | AAAA |
| ATOM | 1723 | C | ASN | 217 | 22.311 | 19.296 | 63.630 | 1.00 | 17.65 | AAAA |
| ATOM | 1724 | O | ASN | 217 | 21.381 | 18.550 | 63.894 | 1.00 | 17.63 | AAAA |
| ATOM | 1725 | N | LEU | 218 | 22.236 | 20.610 | 63.793 | 1.00 | 21.68 | AAAA |
| ATOM | 1726 | CA | LEU | 218 | 21.014 | 21.197 | 64.320 | 1.00 | 21.20 | AAAA |
| ATOM | 1727 | CB | LEU | 218 | 21.186 | 21.547 | 65.808 | 1.00 | 17.73 | AAAA |
| ATOM | 1728 | CG | LEU | 218 | 19.906 | 21.702 | 66.647 | 1.00 | 32.30 | AAAA |
| ATOM | 1729 | CD1 | LEU | 218 | 20.228 | 22.427 | 67.944 | 1.00 | 24.51 | AAAA |
| ATOM | 1730 | CD2 | LEU | 218 | 18.862 | 22.464 | 65.903 | 1.00 | 40.08 | AAAA |
| ATOM | 1731 | C | LEU | 218 | 20.700 | 22.459 | 63.554 | 1.00 | 19.46 | AAAA |
| ATOM | 1732 | O | LEU | 218 | 21.467 | 23.425 | 63.615 | 1.00 | 16.70 | AAAA |
| ATOM | 1733 | N | ASN | 219 | 19.590 | 22.441 | 62.824 | 1.00 | 15.43 | AAAA |
| ATOM | 1734 | CA | ASN | 219 | 19.143 | 23.609 | 62.072 | 1.00 | 14.05 | AAAA |
| ATOM | 1735 | CB | ASN | 219 | 18.634 | 23.232 | 60.665 | 1.00 | 15.92 | AAAA |
| ATOM | 1736 | CG | ASN | 219 | 19.732 | 22.738 | 59.750 | 1.00 | 22.73 | AAAA |
| ATOM | 1737 | OD1 | ASN | 219 | 20.861 | 23.232 | 59.802 | 1.00 | 17.90 | AAAA |
| ATOM | 1738 | ND2 | ASN | 219 | 19.398 | 21.789 | 58.868 | 1.00 | 16.62 | AAAA |
| ATOM | 1739 | C | ASN | 219 | 17.990 | 24.256 | 62.821 | 1.00 | 21.98 | AAAA |
| ATOM | 1740 | O | ASN | 219 | 17.075 | 23.569 | 63.262 | 1.00 | 18.65 | AAAA |
| ATOM | 1741 | N | ILE | 220 | 18.025 | 25.580 | 62.952 | 1.00 | 16.82 | AAAA |
| ATOM | 1742 | CA | ILE | 220 | 16.951 | 26.298 | 63.640 | 1.00 | 13.22 | AAAA |
| ATOM | 1743 | CB | ILE | 220 | 17.522 | 27.115 | 64.823 | 1.00 | 15.70 | AAAA |
| ATOM | 1744 | CG2 | ILE | 220 | 16.411 | 27.912 | 65.479 | 1.00 | 15.18 | AAAA |
| ATOM | 1745 | CG1 | ILE | 220 | 18.246 | 26.193 | 65.823 | 1.00 | 19.11 | AAAA |
| ATOM | 1746 | CD1 | ILE | 220 | 17.350 | 25.259 | 66.632 | 1.00 | 22.75 | AAAA |
| ATOM | 1747 | C | ILE | 220 | 16.363 | 27.246 | 62.573 | 1.00 | 18.80 | AAAA |
| ATOM | 1748 | O | ILE | 220 | 16.810 | 28.386 | 62.419 | 1.00 | 15.52 | AAAA |
| ATOM | 1749 | N | PRO | 221 | 15.341 | 26.790 | 61.826 | 1.00 | 16.72 | AAAA |
| ATOM | 1750 | CD | PRO | 221 | 14.612 | 25.518 | 61.906 | 1.00 | 18.83 | AAAA |
| ATOM | 1751 | CA | PRO | 221 | 14.739 | 27.628 | 60.785 | 1.00 | 19.83 | AAAA |
| ATOM | 1752 | CB | PRO | 221 | 13.930 | 26.615 | 59.948 | 1.00 | 20.76 | AAAA |
| ATOM | 1753 | CG | PRO | 221 | 14.409 | 25.241 | 60.462 | 1.00 | 28.73 | AAAA |
| ATOM | 1754 | C | PRO | 221 | 13.849 | 28.664 | 61.444 | 1.00 | 21.26 | AAAA |
| ATOM | 1755 | O | PRO | 221 | 13.061 | 28.318 | 62.314 | 1.00 | 22.46 | AAAA |
| ATOM | 1756 | N | LEU | 222 | 13.977 | 29.926 | 61.028 | 1.00 | 19.70 | AAAA |
| ATOM | 1757 | CA | LEU | 222 | 13.209 | 31.018 | 61.612 | 1.00 | 21.62 | AAAA |
| ATOM | 1758 | CB | LEU | 222 | 14.163 | 31.972 | 62.319 | 1.00 | 16.46 | AAAA |
| ATOM | 1759 | CG | LEU | 222 | 14.868 | 31.232 | 63.466 | 1.00 | 18.65 | AAAA |
| ATOM | 1760 | CD1 | LEU | 222 | 16.026 | 32.072 | 64.014 | 1.00 | 21.32 | AAAA |
| ATOM | 1761 | CD2 | LEU | 222 | 13.857 | 30.925 | 64.555 | 1.00 | 19.98 | AAAA |
| ATOM | 1762 | C | LEU | 222 | 12.350 | 31.763 | 60.590 | 1.00 | 19.68 | AAAA |
| ATOM | 1763 | O | LEU | 222 | 12.687 | 31.830 | 59.412 | 1.00 | 18.07 | AAAA |
| ATOM | 1764 | N | PRO | 223 | 11.220 | 32.329 | 61.042 | 1.00 | 19.37 | AAAA |
| ATOM | 1765 | CD | PRO | 223 | 10.723 | 32.249 | 62.431 | 1.00 | 17.38 | AAAA |
| ATOM | 1766 | CA | PRO | 223 | 10.264 | 33.065 | 60.203 | 1.00 | 19.59 | AAAA |
| ATOM | 1767 | CB | PRO | 223 | 9.006 | 33.083 | 61.074 | 1.00 | 20.08 | AAAA |
| ATOM | 1768 | CG | PRO | 223 | 9.608 | 33.304 | 62.441 | 1.00 | 21.96 | AAAA |
| ATOM | 1769 | C | PRO | 223 | 10.606 | 34.458 | 59.723 | 1.00 | 23.15 | AAAA |
| ATOM | 1770 | O | PRO | 223 | 11.525 | 35.101 | 60.214 | 1.00 | 15.81 | AAAA |
| ATOM | 1771 | N | LYS | 224 | 9.830 | 34.912 | 58.745 | 1.00 | 16.41 | AAAA |
| ATOM | 1772 | CA | LYS | 224 | 9.975 | 36.254 | 58.200 | 1.00 | 16.11 | AAAA |
| ATOM | 1773 | CB | LYS | 224 | 9.002 | 36.446 | 57.039 | 1.00 | 20.34 | AAAA |
| ATOM | 1774 | CG | LYS | 224 | 9.163 | 35.441 | 55.900 | 1.00 | 19.33 | AAAA |
| ATOM | 1775 | CD | LYS | 224 | 8.109 | 35.687 | 54.807 | 1.00 | 25.49 | AAAA |
| ATOM | 1776 | CE | LYS | 224 | 8.209 | 34.624 | 53.704 | 1.00 | 24.14 | AAAA |
| ATOM | 1777 | NZ | LYS | 224 | 7.207 | 34.843 | 52.618 | 1.00 | 34.08 | AAAA |
| ATOM | 1778 | C | LYS | 224 | 9.638 | 37.289 | 59.284 | 1.00 | 15.77 | AAAA |
| ATOM | 1779 | O | LYS | 224 | 8.819 | 37.032 | 60.186 | 1.00 | 21.07 | AAAA |
| ATOM | 1780 | N | GLY | 225 | 10.239 | 38.469 | 59.171 | 1.00 | 20.77 | AAAA |
| ATOM | 1781 | CA | GLY | 225 | 9.974 | 39.527 | 60.129 | 1.00 | 20.30 | AAAA |
| ATOM | 1782 | C | GLY | 225 | 10.556 | 39.286 | 61.507 | 1.00 | 20.63 | AAAA |

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Figure 16-28

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1783 | O | GLY | 225 | 10.128 | 39.912 | 62.468 | 1.00 | 20.66 | AAAA |
| ATOM | 1784 | N | LEU | 226 | 11.540 | 38.395 | 61.606 | 1.00 | 20.37 | AAAA |
| ATOM | 1785 | CA | LEU | 226 | 12.154 | 38.063 | 62.893 | 1.00 | 18.71 | AAAA |
| ATOM | 1786 | CB | LEU | 226 | 13.354 | 37.145 | 62.670 | 1.00 | 13.63 | AAAA |
| ATOM | 1787 | CG | LEU | 226 | 13.836 | 36.443 | 63.939 | 1.00 | 18.44 | AAAA |
| ATOM | 1788 | CD1 | LEU | 226 | 12.834 | 35.329 | 64.243 | 1.00 | 18.09 | AAAA |
| ATOM | 1789 | CD2 | LEU | 226 | 15.232 | 35.844 | 63.741 | 1.00 | 17.96 | AAAA |
| ATOM | 1790 | C | LEU | 226 | 12.649 | 39.309 | 63.642 | 1.00 | 19.84 | AAAA |
| ATOM | 1791 | O | LEU | 226 | 13.320 | 40.151 | 63.052 | 1.00 | 18.13 | AAAA |
| ATOM | 1792 | N | ASN | 227 | 12.336 | 39.421 | 64.932 | 1.00 | 23.30 | AAAA |
| ATOM | 1793 | CA | ASN | 227 | 12.815 | 40.571 | 65.692 | 1.00 | 20.88 | AAAA |
| ATOM | 1794 | CB | ASN | 227 | 11.682 | 41.261 | 66.485 | 1.00 | 21.73 | AAAA |
| ATOM | 1795 | CG | ASN | 227 | 11.061 | 40.368 | 67.546 | 1.00 | 20.47 | AAAA |
| ATOM | 1796 | OD1 | ASN | 227 | 11.762 | 39.736 | 68.341 | 1.00 | 23.80 | AAAA |
| ATOM | 1797 | ND2 | ASN | 227 | 9.729 | 40.340 | 67.581 | 1.00 | 21.08 | AAAA |
| ATOM | 1798 | C | ASN | 227 | 13.950 | 40.152 | 66.612 | 1.00 | 25.24 | AAAA |
| ATOM | 1799 | O | ASN | 227 | 14.282 | 38.965 | 66.702 | 1.00 | 18.54 | AAAA |
| ATOM | 1800 | N | ASP | 228 | 14.547 | 41.124 | 67.296 | 1.00 | 19.41 | AAAA |
| ATOM | 1801 | CA | ASP | 228 | 15.682 | 40.844 | 68.169 | 1.00 | 22.15 | AAAA |
| ATOM | 1802 | CB | ASP | 228 | 16.208 | 42.141 | 68.802 | 1.00 | 16.82 | AAAA |
| ATOM | 1803 | CG | ASP | 228 | 16.852 | 43.060 | 67.796 | 1.00 | 30.68 | AAAA |
| ATOM | 1804 | OD1 | ASP | 228 | 17.182 | 42.576 | 66.690 | 1.00 | 23.87 | AAAA |
| ATOM | 1805 | OD2 | ASP | 228 | 17.053 | 44.256 | 68.123 | 1.00 | 25.02 | AAAA |
| ATOM | 1806 | C | ASP | 228 | 15.440 | 39.835 | 69.265 | 1.00 | 18.83 | AAAA |
| ATOM | 1807 | O | ASP | 228 | 16.298 | 39.002 | 69.536 | 1.00 | 16.28 | AAAA |
| ATOM | 1808 | N | ASN | 229 | 14.291 | 39.930 | 69.928 | 1.00 | 20.73 | AAAA |
| ATOM | 1809 | CA | ASN | 229 | 13.975 | 39.015 | 71.007 | 1.00 | 21.75 | AAAA |
| ATOM | 1810 | CB | ASN | 229 | 12.706 | 39.483 | 71.712 | 1.00 | 19.46 | AAAA |
| ATOM | 1811 | CG | ASN | 229 | 12.943 | 40.738 | 72.516 | 1.00 | 27.14 | AAAA |
| ATOM | 1812 | OD1 | ASN | 229 | 13.588 | 40.691 | 73.556 | 1.00 | 33.03 | AAAA |
| ATOM | 1813 | ND2 | ASN | 229 | 12.464 | 41.874 | 72.019 | 1.00 | 21.35 | AAAA |
| ATOM | 1814 | C | ASN | 229 | 13.833 | 37.596 | 70.503 | 1.00 | 18.47 | AAAA |
| ATOM | 1815 | O | ASN | 229 | 14.284 | 36.644 | 71.151 | 1.00 | 22.47 | AAAA |
| ATOM | 1816 | N | GLU | 230 | 13.252 | 37.454 | 69.319 | 1.00 | 17.79 | AAAA |
| ATOM | 1817 | CA | GLU | 230 | 13.081 | 36.125 | 68.748 | 1.00 | 21.18 | AAAA |
| ATOM | 1818 | CB | GLU | 230 | 12.152 | 36.193 | 67.536 | 1.00 | 20.54 | AAAA |
| ATOM | 1819 | CG | GLU | 230 | 10.765 | 36.714 | 67.890 | 1.00 | 28.98 | AAAA |
| ATOM | 1820 | CD | GLU | 230 | 9.870 | 36.816 | 66.677 | 1.00 | 24.35 | AAAA |
| ATOM | 1821 | OE1 | GLU | 230 | 10.360 | 37.296 | 65.638 | 1.00 | 22.00 | AAAA |
| ATOM | 1822 | OE2 | GLU | 230 | 8.683 | 36.443 | 66.772 | 1.00 | 24.99 | AAAA |
| ATOM | 1823 | C | GLU | 230 | 14.422 | 35.507 | 68.361 | 1.00 | 16.89 | AAAA |
| ATOM | 1824 | O | GLU | 230 | 14.663 | 34.326 | 68.603 | 1.00 | 19.45 | AAAA |
| ATOM | 1825 | N | PHE | 231 | 15.305 | 36.305 | 67.772 | 1.00 | 15.68 | AAAA |
| ATOM | 1826 | CA | PHE | 231 | 16.616 | 35.788 | 67.389 | 1.00 | 15.78 | AAAA |
| ATOM | 1827 | CB | PHE | 231 | 17.420 | 36.863 | 66.649 | 1.00 | 13.22 | AAAA |
| ATOM | 1828 | CG | PHE | 231 | 18.719 | 36.361 | 66.069 | 1.00 | 20.63 | AAAA |
| ATOM | 1829 | CD1 | PHE | 231 | 18.723 | 35.445 | 65.016 | 1.00 | 18.42 | AAAA |
| ATOM | 1830 | CD2 | PHE | 231 | 19.936 | 36.804 | 66.568 | 1.00 | 21.10 | AAAA |
| ATOM | 1831 | CE1 | PHE | 231 | 19.918 | 34.983 | 64.471 | 1.00 | 17.67 | AAAA |
| ATOM | 1832 | CE2 | PHE | 231 | 21.144 | 36.346 | 66.029 | 1.00 | 28.29 | AAAA |
| ATOM | 1833 | CZ | PHE | 231 | 21.130 | 35.431 | 64.976 | 1.00 | 27.85 | AAAA |
| ATOM | 1834 | C | PHE | 231 | 17.385 | 35.332 | 68.636 | 1.00 | 18.54 | AAAA |
| ATOM | 1835 | O | PHE | 231 | 17.869 | 34.201 | 68.702 | 1.00 | 18.86 | AAAA |
| ATOM | 1836 | N | LEU | 232 | 17.495 | 36.204 | 69.636 | 1.00 | 19.07 | AAAA |
| ATOM | 1837 | CA | LEU | 232 | 18.239 | 35.850 | 70.848 | 1.00 | 17.39 | AAAA |
| ATOM | 1838 | CB | LEU | 232 | 18.415 | 37.078 | 71.737 | 1.00 | 24.53 | AAAA |
| ATOM | 1839 | CG | LEU | 232 | 19.214 | 38.202 | 71.061 | 1.00 | 16.64 | AAAA |
| ATOM | 1840 | CD1 | LEU | 232 | 19.134 | 39.449 | 71.934 | 1.00 | 26.70 | AAAA |
| ATOM | 1841 | CD2 | LEU | 232 | 20.659 | 37.806 | 70.810 | 1.00 | 18.77 | AAAA |
| ATOM | 1842 | C | LEU | 232 | 17.607 | 34.707 | 71.628 | 1.00 | 19.82 | AAAA |
| ATOM | 1843 | O | LEU | 232 | 18.309 | 33.904 | 72.217 | 1.00 | 21.80 | AAAA |
| ATOM | 1844 | N | PHE | 233 | 16.281 | 34.640 | 71.648 | 1.00 | 17.18 | AAAA |
| ATOM | 1845 | CA | PHE | 233 | 15.587 | 33.537 | 72.309 | 1.00 | 23.34 | AAAA |
| ATOM | 1846 | CB | PHE | 233 | 14.074 | 33.663 | 72.095 | 1.00 | 19.17 | AAAA |
| ATOM | 1847 | CG | PHE | 233 | 13.289 | 32.447 | 72.523 | 1.00 | 21.40 | AAAA |
| ATOM | 1848 | CD1 | PHE | 233 | 12.863 | 32.302 | 73.841 | 1.00 | 29.62 | AAAA |

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Figure 16-29

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1849 | CD2 | PHE | 233 | 12.942 | 31.473 | 71.596 | 1.00 | 19.92 | AAAA |
| ATOM | 1850 | CE1 | PHE | 233 | 12.088 | 31.206 | 74.229 | 1.00 | 29.35 | AAAA |
| ATOM | 1851 | CE2 | PHE | 233 | 12.168 | 30.363 | 71.966 | 1.00 | 25.37 | AAAA |
| ATOM | 1852 | CZ | PHE | 233 | 11.737 | 30.231 | 73.283 | 1.00 | 30.28 | AAAA |
| ATOM | 1853 | C | PHE | 233 | 16.041 | 32.234 | 71.660 | 1.00 | 23.12 | AAAA |
| ATOM | 1854 | O | PHE | 233 | 16.433 | 31.273 | 72.332 | 1.00 | 18.35 | AAAA |
| ATOM | 1855 | N | ALA | 234 | 15.961 | 32.208 | 70.332 | 1.00 | 17.26 | AAAA |
| ATOM | 1856 | CA | ALA | 234 | 16.332 | 31.026 | 69.562 | 1.00 | 17.67 | AAAA |
| ATOM | 1857 | CB | ALA | 234 | 16.085 | 31.297 | 68.046 | 1.00 | 19.08 | AAAA |
| ATOM | 1858 | C | ALA | 234 | 17.786 | 30.641 | 69.800 | 1.00 | 16.31 | AAAA |
| ATOM | 1859 | O | ALA | 234 | 18.127 | 29.461 | 69.926 | 1.00 | 16.75 | AAAA |
| ATOM | 1860 | N | LEU | 235 | 18.646 | 31.643 | 69.846 | 1.00 | 16.73 | AAAA |
| ATOM | 1861 | CA | LEU | 235 | 20.074 | 31.411 | 70.051 | 1.00 | 19.14 | AAAA |
| ATOM | 1862 | CB | LEU | 235 | 20.823 | 32.742 | 69.956 | 1.00 | 21.72 | AAAA |
| ATOM | 1863 | CG | LEU | 235 | 22.226 | 32.790 | 69.345 | 1.00 | 36.73 | AAAA |
| ATOM | 1864 | CD1 | LEU | 235 | 23.026 | 33.844 | 70.105 | 1.00 | 20.69 | AAAA |
| ATOM | 1865 | CD2 | LEU | 235 | 22.917 | 31.426 | 69.393 | 1.00 | 22.96 | AAAA |
| ATOM | 1866 | C | LEU | 235 | 20.354 | 30.776 | 71.421 | 1.00 | 18.71 | AAAA |
| ATOM | 1867 | O | LEU | 235 | 21.028 | 29.747 | 71.522 | 1.00 | 18.59 | AAAA |
| ATOM | 1868 | N | GLU | 236 | 19.831 | 31.390 | 72.479 | 1.00 | 25.43 | AAAA |
| ATOM | 1869 | CA | GLU | 236 | 20.046 | 30.883 | 73.839 | 1.00 | 19.75 | AAAA |
| ATOM | 1870 | CB | GLU | 236 | 19.335 | 31.777 | 74.860 | 1.00 | 23.18 | AAAA |
| ATOM | 1871 | CG | GLU | 236 | 19.725 | 33.229 | 74.777 | 1.00 | 38.53 | AAAA |
| ATOM | 1872 | CD | GLU | 236 | 18.857 | 34.119 | 75.648 | 1.00 | 42.42 | AAAA |
| ATOM | 1873 | OE1 | GLU | 236 | 17.617 | 34.171 | 75.428 | 1.00 | 45.43 | AAAA |
| ATOM | 1874 | OE2 | GLU | 236 | 19.425 | 34.768 | 76.548 | 1.00 | 48.76 | AAAA |
| ATOM | 1875 | C | GLU | 236 | 19.541 | 29.452 | 74.011 | 1.00 | 25.85 | AAAA |
| ATOM | 1876 | O | GLU | 236 | 20.222 | 28.603 | 74.597 | 1.00 | 21.36 | AAAA |
| ATOM | 1877 | N | LYS | 237 | 18.343 | 29.193 | 73.501 | 1.00 | 23.16 | AAAA |
| ATOM | 1878 | CA | LYS | 237 | 17.752 | 27.871 | 73.610 | 1.00 | 17.06 | AAAA |
| ATOM | 1879 | CB | LYS | 237 | 16.282 | 27.943 | 73.193 | 1.00 | 26.98 | AAAA |
| ATOM | 1880 | CG | LYS | 237 | 15.483 | 26.711 | 73.519 | 1.00 | 52.00 | AAAA |
| ATOM | 1881 | CD | LYS | 237 | 14.078 | 27.110 | 73.932 | 1.00 | 56.40 | AAAA |
| ATOM | 1882 | CE | LYS | 237 | 14.131 | 27.979 | 75.183 | 1.00 | 52.03 | AAAA |
| ATOM | 1883 | NZ | LYS | 237 | 12.782 | 28.421 | 75.614 | 1.00 | 55.53 | AAAA |
| ATOM | 1884 | C | LYS | 237 | 18.502 | 26.827 | 72.785 | 1.00 | 18.46 | AAAA |
| ATOM | 1885 | O | LYS | 237 | 18.691 | 25.692 | 73.231 | 1.00 | 21.20 | AAAA |
| ATOM | 1886 | N | SER | 238 | 18.932 | 27.187 | 71.578 | 1.00 | 21.28 | AAAA |
| ATOM | 1887 | CA | SER | 238 | 19.649 | 26.208 | 70.776 | 1.00 | 16.47 | AAAA |
| ATOM | 1888 | CB | SER | 238 | 19.745 | 26.666 | 69.307 | 1.00 | 19.75 | AAAA |
| ATOM | 1889 | OG | SER | 238 | 20.475 | 27.858 | 69.160 | 1.00 | 22.52 | AAAA |
| ATOM | 1890 | C | SER | 238 | 21.039 | 25.923 | 71.361 | 1.00 | 18.79 | AAAA |
| ATOM | 1891 | O | SER | 238 | 21.521 | 24.788 | 71.312 | 1.00 | 20.60 | AAAA |
| ATOM | 1892 | N | LEU | 239 | 21.690 | 26.937 | 71.925 | 1.00 | 22.95 | AAAA |
| ATOM | 1893 | CA | LEU | 239 | 23.004 | 26.701 | 72.513 | 1.00 | 20.98 | AAAA |
| ATOM | 1894 | CB | LEU | 239 | 23.652 | 28.008 | 72.986 | 1.00 | 18.39 | AAAA |
| ATOM | 1895 | CG | LEU | 239 | 23.985 | 29.072 | 71.933 | 1.00 | 20.02 | AAAA |
| ATOM | 1896 | CD1 | LEU | 239 | 24.538 | 30.311 | 72.636 | 1.00 | 27.02 | AAAA |
| ATOM | 1897 | CD2 | LEU | 239 | 25.010 | 28.556 | 70.933 | 1.00 | 20.31 | AAAA |
| ATOM | 1898 | C | LEU | 239 | 22.882 | 25.735 | 73.680 | 1.00 | 25.16 | AAAA |
| ATOM | 1899 | O | LEU | 239 | 23.780 | 24.929 | 73.920 | 1.00 | 20.70 | AAAA |
| ATOM | 1900 | N | GLU | 240 | 21.768 | 25.800 | 74.398 | 1.00 | 24.93 | AAAA |
| ATOM | 1901 | CA | GLU | 240 | 21.570 | 24.912 | 75.536 | 1.00 | 25.72 | AAAA |
| ATOM | 1902 | CB | GLU | 240 | 20.331 | 25.356 | 76.337 | 1.00 | 29.10 | AAAA |
| ATOM | 1903 | CG | GLU | 240 | 20.042 | 24.531 | 77.581 | 1.00 | 49.56 | AAAA |
| ATOM | 1904 | CD | GLU | 240 | 19.053 | 25.212 | 78.515 | 1.00 | 63.15 | AAAA |
| ATOM | 1905 | OE1 | GLU | 240 | 17.935 | 25.550 | 78.067 | 1.00 | 69.26 | AAAA |
| ATOM | 1906 | OE2 | GLU | 240 | 19.400 | 25.410 | 79.703 | 1.00 | 66.68 | AAAA |
| ATOM | 1907 | C | GLU | 240 | 21.440 | 23.469 | 75.046 | 1.00 | 23.44 | AAAA |
| ATOM | 1908 | O | GLU | 240 | 21.951 | 22.535 | 75.674 | 1.00 | 23.10 | AAAA |
| ATOM | 1909 | N | ILE | 241 | 20.771 | 23.294 | 73.913 | 1.00 | 19.52 | AAAA |
| ATOM | 1910 | CA | ILE | 241 | 20.598 | 21.978 | 73.321 | 1.00 | 24.06 | AAAA |
| ATOM | 1911 | CB | ILE | 241 | 19.705 | 22.039 | 72.052 | 1.00 | 23.80 | AAAA |
| ATOM | 1912 | CG2 | ILE | 241 | 19.718 | 20.678 | 71.323 | 1.00 | 24.94 | AAAA |
| ATOM | 1913 | CG1 | ILE | 241 | 18.281 | 22.433 | 72.439 | 1.00 | 28.60 | AAAA |
| ATOM | 1914 | CD1 | ILE | 241 | 17.336 | 22.600 | 71.257 | 1.00 | 27.04 | AAAA |

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Figure 16-30

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1915 | C | ILE | 241 | 21.957 | 21.404 | 72.941 | 1.00 | 25.48 | AAAA |
| ATOM | 1916 | O | ILE | 241 | 22.244 | 20.234 | 73.195 | 1.00 | 19.43 | AAAA |
| ATOM | 1917 | N | VAL | 242 | 22.799 | 22.235 | 72.334 | 1.00 | 20.41 | AAAA |
| ATOM | 1918 | CA | VAL | 242 | 24.116 | 21.782 | 71.928 | 1.00 | 23.17 | AAAA |
| ATOM | 1919 | CB | VAL | 242 | 24.853 | 22.856 | 71.107 | 1.00 | 26.48 | AAAA |
| ATOM | 1920 | CG1 | VAL | 242 | 26.273 | 22.394 | 70.807 | 1.00 | 18.67 | AAAA |
| ATOM | 1921 | CG2 | VAL | 242 | 24.093 | 23.135 | 69.802 | 1.00 | 26.97 | AAAA |
| ATOM | 1922 | C | VAL | 242 | 24.962 | 21.456 | 73.154 | 1.00 | 24.81 | AAAA |
| ATOM | 1923 | O | VAL | 242 | 25.566 | 20.384 | 73.235 | 1.00 | 22.49 | AAAA |
| ATOM | 1924 | N | LYS | 243 | 24.989 | 22.387 | 74.102 | 1.00 | 26.06 | AAAA |
| ATOM | 1925 | CA | LYS | 243 | 25.775 | 22.202 | 75.311 | 1.00 | 32.57 | AAAA |
| ATOM | 1926 | CB | LYS | 243 | 25.599 | 23.379 | 76.272 | 1.00 | 28.53 | AAAA |
| ATOM | 1927 | CG | LYS | 243 | 26.386 | 23.183 | 77.568 | 1.00 | 43.21 | AAAA |
| ATOM | 1928 | CD | LYS | 243 | 26.022 | 24.191 | 78.653 | 1.00 | 53.10 | AAAA |
| ATOM | 1929 | CE | LYS | 243 | 26.407 | 25.607 | 78.287 | 1.00 | 50.30 | AAAA |
| ATOM | 1930 | NZ | LYS | 243 | 26.045 | 26.548 | 79.389 | 1.00 | 59.15 | AAAA |
| ATOM | 1931 | C | LYS | 243 | 25.433 | 20.917 | 76.046 | 1.00 | 30.38 | AAAA |
| ATOM | 1932 | O | LYS | 243 | 26.321 | 20.255 | 76.578 | 1.00 | 35.44 | AAAA |
| ATOM | 1933 | N | GLU | 244 | 24.161 | 20.542 | 76.076 | 1.00 | 28.12 | AAAA |
| ATOM | 1934 | CA | GLU | 244 | 23.798 | 19.320 | 76.798 | 1.00 | 37.54 | AAAA |
| ATOM | 1935 | CB | GLU | 244 | 22.288 | 19.260 | 77.048 | 1.00 | 35.34 | AAAA |
| ATOM | 1936 | CG | GLU | 244 | 21.735 | 20.459 | 77.816 | 1.00 | 55.88 | AAAA |
| ATOM | 1937 | CD | GLU | 244 | 20.281 | 20.275 | 78.230 | 1.00 | 57.89 | AAAA |
| ATOM | 1938 | OE1 | GLU | 244 | 19.673 | 21.246 | 78.738 | 1.00 | 60.60 | AAAA |
| ATOM | 1939 | OE2 | GLU | 244 | 19.753 | 19.152 | 78.062 | 1.00 | 57.73 | AAAA |
| ATOM | 1940 | C | GLU | 244 | 24.231 | 18.034 | 76.102 | 1.00 | 38.17 | AAAA |
| ATOM | 1941 | O | GLU | 244 | 24.294 | 16.978 | 76.727 | 1.00 | 38.46 | AAAA |
| ATOM | 1942 | N | VAL | 245 | 24.541 | 18.124 | 74.817 | 1.00 | 30.29 | AAAA |
| ATOM | 1943 | CA | VAL | 245 | 24.933 | 16.958 | 74.042 | 1.00 | 29.17 | AAAA |
| ATOM | 1944 | CB | VAL | 245 | 23.984 | 16.778 | 72.833 | 1.00 | 46.68 | AAAA |
| ATOM | 1945 | CG1 | VAL | 245 | 24.462 | 15.641 | 71.942 | 1.00 | 53.09 | AAAA |
| ATOM | 1946 | CG2 | VAL | 245 | 22.581 | 16.488 | 73.327 | 1.00 | 54.19 | AAAA |
| ATOM | 1947 | C | VAL | 245 | 26.364 | 16.982 | 73.508 | 1.00 | 34.90 | AAAA |
| ATOM | 1948 | O | VAL | 245 | 26.915 | 15.939 | 73.164 | 1.00 | 34.73 | AAAA |
| ATOM | 1949 | N | PHE | 246 | 26.980 | 18.156 | 73.465 | 1.00 | 29.22 | AAAA |
| ATOM | 1950 | CA | PHE | 246 | 28.324 | 18.256 | 72.897 | 1.00 | 29.17 | AAAA |
| ATOM | 1951 | CB | PHE | 246 | 28.178 | 18.800 | 71.464 | 1.00 | 30.42 | AAAA |
| ATOM | 1952 | CG | PHE | 246 | 29.384 | 18.588 | 70.585 | 1.00 | 25.62 | AAAA |
| ATOM | 1953 | CD1 | PHE | 246 | 29.695 | 17.326 | 70.097 | 1.00 | 28.89 | AAAA |
| ATOM | 1954 | CD2 | PHE | 246 | 30.167 | 19.668 | 70.196 | 1.00 | 25.17 | AAAA |
| ATOM | 1955 | CE1 | PHE | 246 | 30.771 | 17.138 | 69.222 | 1.00 | 23.43 | AAAA |
| ATOM | 1956 | CE2 | PHE | 246 | 31.248 | 19.495 | 69.322 | 1.00 | 22.40 | AAAA |
| ATOM | 1957 | CZ | PHE | 246 | 31.549 | 18.236 | 68.835 | 1.00 | 19.88 | AAAA |
| ATOM | 1958 | C | PHE | 246 | 29.233 | 19.176 | 73.712 | 1.00 | 23.38 | AAAA |
| ATOM | 1959 | O | PHE | 246 | 28.867 | 20.312 | 74.002 | 1.00 | 29.15 | AAAA |
| ATOM | 1960 | N | GLU | 247 | 30.410 | 18.682 | 74.094 | 1.00 | 29.73 | AAAA |
| ATOM | 1961 | CA | GLU | 247 | 31.395 | 19.481 | 74.841 | 1.00 | 28.10 | AAAA |
| ATOM | 1962 | CB | GLU | 247 | 31.912 | 18.726 | 76.074 | 1.00 | 35.75 | AAAA |
| ATOM | 1963 | CG | GLU | 247 | 30.972 | 18.707 | 77.286 | 1.00 | 60.78 | AAAA |
| ATOM | 1964 | CD | GLU | 247 | 29.700 | 17.892 | 77.077 | 1.00 | 70.07 | AAAA |
| ATOM | 1965 | OE1 | GLU | 247 | 28.913 | 18.220 | 76.165 | 1.00 | 79.95 | AAAA |
| ATOM | 1966 | OE2 | GLU | 247 | 29.481 | 16.920 | 77.835 | 1.00 | 76.80 | AAAA |
| ATOM | 1967 | C | GLU | 247 | 32.554 | 19.741 | 73.876 | 1.00 | 28.90 | AAAA |
| ATOM | 1968 | O | GLU | 247 | 33.490 | 18.946 | 73.778 | 1.00 | 23.67 | AAAA |
| ATOM | 1969 | N | PRO | 248 | 32.531 | 20.891 | 73.181 | 1.00 | 25.02 | AAAA |
| ATOM | 1970 | CD | PRO | 248 | 31.574 | 22.003 | 73.310 | 1.00 | 27.23 | AAAA |
| ATOM | 1971 | CA | PRO | 248 | 33.566 | 21.249 | 72.209 | 1.00 | 28.06 | AAAA |
| ATOM | 1972 | CB | PRO | 248 | 33.050 | 22.575 | 71.639 | 1.00 | 28.11 | AAAA |
| ATOM | 1973 | CG | PRO | 248 | 31.551 | 22.512 | 71.897 | 1.00 | 34.57 | AAAA |
| ATOM | 1974 | C | PRO | 248 | 34.968 | 21.416 | 72.770 | 1.00 | 23.87 | AAAA |
| ATOM | 1975 | O | PRO | 248 | 35.132 | 21.897 | 73.887 | 1.00 | 24.05 | AAAA |
| ATOM | 1976 | N | GLU | 249 | 35.965 | 21.013 | 71.983 | 1.00 | 24.34 | AAAA |
| ATOM | 1977 | CA | GLU | 249 | 37.366 | 21.195 | 72.355 | 1.00 | 25.98 | AAAA |
| ATOM | 1978 | CB | GLU | 249 | 38.275 | 20.166 | 71.679 | 1.00 | 22.07 | AAAA |
| ATOM | 1979 | CG | GLU | 249 | 38.046 | 18.726 | 72.116 | 1.00 | 33.40 | AAAA |
| ATOM | 1980 | CD | GLU | 249 | 39.005 | 17.767 | 71.445 | 1.00 | 29.15 | AAAA |

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Figure 16-31

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1981 | OE1 | GLU | 249 | 39.071 | 17.770 | 70.199 | 1.00 | 27.62 | AAAA |
| ATOM | 1982 | OE2 | GLU | 249 | 39.694 | 17.004 | 72.161 | 1.00 | 26.19 | AAAA |
| ATOM | 1983 | C | GLU | 249 | 37.692 | 22.561 | 71.786 | 1.00 | 26.04 | AAAA |
| ATOM | 1984 | O | GLU | 249 | 38.582 | 23.271 | 72.262 | 1.00 | 26.39 | AAAA |
| ATOM | 1985 | N | VAL | 250 | 36.953 | 22.921 | 70.744 | 1.00 | 23.83 | AAAA |
| ATOM | 1986 | CA | VAL | 250 | 37.151 | 24.197 | 70.086 | 1.00 | 19.67 | AAAA |
| ATOM | 1987 | CB | VAL | 250 | 38.438 | 24.178 | 69.210 | 1.00 | 20.88 | AAAA |
| ATOM | 1988 | CG1 | VAL | 250 | 38.348 | 23.117 | 68.128 | 1.00 | 18.18 | AAAA |
| ATOM | 1989 | CG2 | VAL | 250 | 38.647 | 25.530 | 68.591 | 1.00 | 16.71 | AAAA |
| ATOM | 1990 | C | VAL | 250 | 35.946 | 24.483 | 69.207 | 1.00 | 20.78 | AAAA |
| ATOM | 1991 | O | VAL | 250 | 35.299 | 23.556 | 68.746 | 1.00 | 19.60 | AAAA |
| ATOM | 1992 | N | TYR | 251 | 35.633 | 25.757 | 69.000 | 1.00 | 18.75 | AAAA |
| ATOM | 1993 | CA | TYR | 251 | 34.497 | 26.109 | 68.153 | 1.00 | 22.44 | AAAA |
| ATOM | 1994 | CB | TYR | 251 | 33.261 | 26.437 | 69.022 | 1.00 | 16.57 | AAAA |
| ATOM | 1995 | CG | TYR | 251 | 33.207 | 27.856 | 69.575 | 1.00 | 22.36 | AAAA |
| ATOM | 1996 | CD1 | TYR | 251 | 32.654 | 28.896 | 68.823 | 1.00 | 18.12 | AAAA |
| ATOM | 1997 | CE1 | TYR | 251 | 32.612 | 30.185 | 69.308 | 1.00 | 20.40 | AAAA |
| ATOM | 1998 | CD2 | TYR | 251 | 33.715 | 28.160 | 70.842 | 1.00 | 20.04 | AAAA |
| ATOM | 1999 | CE2 | TYR | 251 | 33.676 | 29.475 | 71.349 | 1.00 | 16.60 | AAAA |
| ATOM | 2000 | CZ | TYR | 251 | 33.128 | 30.473 | 70.573 | 1.00 | 14.68 | AAAA |
| ATOM | 2001 | OH | TYR | 251 | 33.100 | 31.780 | 71.011 | 1.00 | 21.79 | AAAA |
| ATOM | 2002 | C | TYR | 251 | 34.811 | 27.294 | 67.236 | 1.00 | 20.28 | AAAA |
| ATOM | 2003 | O | TYR | 251 | 35.695 | 28.107 | 67.525 | 1.00 | 19.91 | AAAA |
| ATOM | 2004 | N | LEU | 252 | 34.097 | 27.360 | 66.109 | 1.00 | 17.90 | AAAA |
| ATOM | 2005 | CA | LEU | 252 | 34.216 | 28.466 | 65.161 | 1.00 | 18.58 | AAAA |
| ATOM | 2006 | CB | LEU | 252 | 34.679 | 28.001 | 63.767 | 1.00 | 17.55 | AAAA |
| ATOM | 2007 | CG | LEU | 252 | 36.028 | 27.290 | 63.718 | 1.00 | 23.36 | AAAA |
| ATOM | 2008 | CD1 | LEU | 252 | 35.819 | 25.820 | 64.017 | 1.00 | 27.78 | AAAA |
| ATOM | 2009 | CD2 | LEU | 252 | 36.631 | 27.440 | 62.331 | 1.00 | 27.29 | AAAA |
| ATOM | 2010 | C | LEU | 252 | 32.816 | 29.049 | 65.052 | 1.00 | 15.49 | AAAA |
| ATOM | 2011 | O | LEU | 252 | 31.819 | 28.320 | 65.120 | 1.00 | 18.82 | AAAA |
| ATOM | 2012 | N | LEU | 253 | 32.756 | 30.360 | 64.891 | 1.00 | 16.80 | AAAA |
| ATOM | 2013 | CA | LEU | 253 | 31.498 | 31.105 | 64.817 | 1.00 | 17.50 | AAAA |
| ATOM | 2014 | CB | LEU | 253 | 31.379 | 31.987 | 66.073 | 1.00 | 15.49 | AAAA |
| ATOM | 2015 | CG | LEU | 253 | 30.326 | 33.085 | 66.165 | 1.00 | 17.75 | AAAA |
| ATOM | 2016 | CD1 | LEU | 253 | 28.946 | 32.438 | 66.172 | 1.00 | 20.85 | AAAA |
| ATOM | 2017 | CD2 | LEU | 253 | 30.536 | 33.897 | 67.464 | 1.00 | 19.05 | AAAA |
| ATOM | 2018 | C | LEU | 253 | 31.516 | 31.985 | 63.580 | 1.00 | 20.22 | AAAA |
| ATOM | 2019 | O | LEU | 253 | 32.474 | 32.727 | 63.371 | 1.00 | 18.14 | AAAA |
| ATOM | 2020 | N | GLN | 254 | 30.466 | 31.913 | 62.765 | 1.00 | 16.50 | AAAA |
| ATOM | 2021 | CA | GLN | 254 | 30.411 | 32.730 | 61.556 | 1.00 | 16.48 | AAAA |
| ATOM | 2022 | CB | GLN | 254 | 30.085 | 31.863 | 60.312 | 1.00 | 25.58 | AAAA |
| ATOM | 2023 | CG | GLN | 254 | 28.647 | 31.798 | 59.871 | 1.00 | 36.40 | AAAA |
| ATOM | 2024 | CD | GLN | 254 | 28.337 | 32.728 | 58.701 | 1.00 | 33.18 | AAAA |
| ATOM | 2025 | OE1 | GLN | 254 | 28.744 | 32.487 | 57.546 | 1.00 | 21.05 | AAAA |
| ATOM | 2026 | NE2 | GLN | 254 | 27.613 | 33.799 | 58.992 | 1.00 | 22.85 | AAAA |
| ATOM | 2027 | C | GLN | 254 | 29.384 | 33.816 | 61.832 | 1.00 | 16.12 | AAAA |
| ATOM | 2028 | O | GLN | 254 | 28.282 | 33.577 | 62.364 | 1.00 | 13.97 | AAAA |
| ATOM | 2029 | N | LEU | 255 | 29.768 | 35.032 | 61.468 | 1.00 | 14.42 | AAAA |
| ATOM | 2030 | CA | LEU | 255 | 28.988 | 36.215 | 61.763 | 1.00 | 17.99 | AAAA |
| ATOM | 2031 | CB | LEU | 255 | 29.834 | 37.070 | 62.719 | 1.00 | 20.68 | AAAA |
| ATOM | 2032 | CG | LEU | 255 | 30.240 | 36.283 | 63.964 | 1.00 | 22.90 | AAAA |
| ATOM | 2033 | CD1 | LEU | 255 | 31.446 | 36.906 | 64.635 | 1.00 | 29.36 | AAAA |
| ATOM | 2034 | CD2 | LEU | 255 | 29.042 | 36.214 | 64.900 | 1.00 | 14.80 | AAAA |
| ATOM | 2035 | C | LEU | 255 | 28.541 | 37.060 | 60.594 | 1.00 | 19.32 | AAAA |
| ATOM | 2036 | O | LEU | 255 | 28.838 | 38.260 | 60.561 | 1.00 | 21.23 | AAAA |
| ATOM | 2037 | N | GLY | 256 | 27.827 | 36.467 | 59.639 | 1.00 | 17.21 | AAAA |
| ATOM | 2038 | CA | GLY | 256 | 27.347 | 37.259 | 58.516 | 1.00 | 15.64 | AAAA |
| ATOM | 2039 | C | GLY | 256 | 26.413 | 38.348 | 59.028 | 1.00 | 17.31 | AAAA |
| ATOM | 2040 | O | GLY | 256 | 25.717 | 38.150 | 60.027 | 1.00 | 15.62 | AAAA |
| ATOM | 2041 | N | THR | 257 | 26.389 | 39.494 | 58.348 | 1.00 | 19.72 | AAAA |
| ATOM | 2042 | CA | THR | 257 | 25.536 | 40.598 | 58.776 | 1.00 | 19.88 | AAAA |
| ATOM | 2043 | CB | THR | 257 | 26.242 | 41.973 | 58.589 | 1.00 | 14.02 | AAAA |
| ATOM | 2044 | OG1 | THR | 257 | 26.538 | 42.187 | 57.206 | 1.00 | 17.58 | AAAA |
| ATOM | 2045 | CG2 | THR | 257 | 27.543 | 42.009 | 59.392 | 1.00 | 19.67 | AAAA |
| ATOM | 2046 | C | THR | 257 | 24.199 | 40.634 | 58.053 | 1.00 | 20.58 | AAAA |

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Figure 16-32

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2047 | O | THR | 257 | 23.403 | 41.545 | 58.266 | 1.00 | 14.59 | AAAA |
| ATOM | 2048 | N | ASP | 258 | 23.927 | 39.639 | 57.213 | 1.00 | 16.56 | AAAA |
| ATOM | 2049 | CA | ASP | 258 | 22.651 | 39.646 | 56.525 | 1.00 | 16.39 | AAAA |
| ATOM | 2050 | CB | ASP | 258 | 22.604 | 38.611 | 55.388 | 1.00 | 18.38 | AAAA |
| ATOM | 2051 | CG | ASP | 258 | 23.037 | 37.229 | 55.811 | 1.00 | 25.85 | AAAA |
| ATOM | 2052 | OD1 | ASP | 258 | 23.222 | 36.995 | 57.022 | 1.00 | 22.32 | AAAA |
| ATOM | 2053 | OD2 | ASP | 258 | 23.187 | 36.370 | 54.909 | 1.00 | 18.12 | AAAA |
| ATOM | 2054 | C | ASP | 258 | 21.396 | 39.563 | 57.397 | 1.00 | 21.25 | AAAA |
| ATOM | 2055 | O | ASP | 258 | 20.300 | 39.781 | 56.897 | 1.00 | 22.52 | AAAA |
| ATOM | 2056 | N | PRO | 259 | 21.510 | 39.172 | 58.680 | 1.00 | 18.17 | AAAA |
| ATOM | 2057 | CD | PRO | 259 | 22.614 | 38.528 | 59.422 | 1.00 | 25.88 | AAAA |
| ATOM | 2058 | CA | PRO | 259 | 20.281 | 39.139 | 59.482 | 1.00 | 21.24 | AAAA |
| ATOM | 2059 | CB | PRO | 259 | 20.710 | 38.363 | 60.735 | 1.00 | 21.18 | AAAA |
| ATOM | 2060 | CG | PRO | 259 | 22.174 | 38.707 | 60.846 | 1.00 | 36.11 | AAAA |
| ATOM | 2061 | C | PRO | 259 | 19.705 | 40.534 | 59.820 | 1.00 | 20.88 | AAAA |
| ATOM | 2062 | O | PRO | 259 | 18.572 | 40.647 | 60.280 | 1.00 | 19.25 | AAAA |
| ATOM | 2063 | N | LEU | 260 | 20.473 | 41.591 | 59.571 | 1.00 | 18.75 | AAAA |
| ATOM | 2064 | CA | LEU | 260 | 20.023 | 42.949 | 59.875 | 1.00 | 22.16 | AAAA |
| ATOM | 2065 | CB | LEU | 260 | 21.202 | 43.935 | 59.778 | 1.00 | 20.35 | AAAA |
| ATOM | 2066 | CG | LEU | 260 | 22.403 | 43.640 | 60.682 | 1.00 | 21.82 | AAAA |
| ATOM | 2067 | CD1 | LEU | 260 | 23.604 | 44.486 | 60.253 | 1.00 | 18.57 | AAAA |
| ATOM | 2068 | CD2 | LEU | 260 | 22.032 | 43.873 | 62.123 | 1.00 | 19.18 | AAAA |
| ATOM | 2069 | C | LEU | 260 | 18.876 | 43.469 | 59.014 | 1.00 | 24.16 | AAAA |
| ATOM | 2070 | O | LEU | 260 | 18.742 | 43.144 | 57.826 | 1.00 | 21.69 | AAAA |
| ATOM | 2071 | N | LEU | 261 | 18.049 | 44.300 | 59.634 | 1.00 | 19.54 | AAAA |
| ATOM | 2072 | CA | LEU | 261 | 16.903 | 44.913 | 58.965 | 1.00 | 17.34 | AAAA |
| ATOM | 2073 | CB | LEU | 261 | 16.285 | 45.967 | 59.892 | 1.00 | 19.96 | AAAA |
| ATOM | 2074 | CG | LEU | 261 | 15.204 | 46.879 | 59.300 | 1.00 | 29.99 | AAAA |
| ATOM | 2075 | CD1 | LEU | 261 | 14.080 | 46.040 | 58.732 | 1.00 | 33.66 | AAAA |
| ATOM | 2076 | CD2 | LEU | 261 | 14.682 | 47.819 | 60.376 | 1.00 | 44.71 | AAAA |
| ATOM | 2077 | C | LEU | 261 | 17.262 | 45.550 | 57.620 | 1.00 | 18.11 | AAAA |
| ATOM | 2078 | O | LEU | 261 | 16.539 | 45.386 | 56.634 | 1.00 | 19.02 | AAAA |
| ATOM | 2079 | N | GLU | 262 | 18.391 | 46.249 | 57.566 | 1.00 | 22.68 | AAAA |
| ATOM | 2080 | CA | GLU | 262 | 18.802 | 46.921 | 56.338 | 1.00 | 18.46 | AAAA |
| ATOM | 2081 | CB | GLU | 262 | 19.875 | 47.965 | 56.641 | 1.00 | 22.01 | AAAA |
| ATOM | 2082 | CG | GLU | 262 | 19.365 | 49.136 | 57.443 | 1.00 | 22.94 | AAAA |
| ATOM | 2083 | CD | GLU | 262 | 19.434 | 48.902 | 58.927 | 1.00 | 23.11 | AAAA |
| ATOM | 2084 | OE1 | GLU | 262 | 19.668 | 47.748 | 59.357 | 1.00 | 24.58 | AAAA |
| ATOM | 2085 | OE2 | GLU | 262 | 19.238 | 49.883 | 59.667 | 1.00 | 27.06 | AAAA |
| ATOM | 2086 | C | GLU | 262 | 19.281 | 46.034 | 55.197 | 1.00 | 25.65 | AAAA |
| ATOM | 2087 | O | GLU | 262 | 19.446 | 46.510 | 54.070 | 1.00 | 25.49 | AAAA |
| ATOM | 2088 | N | ASP | 263 | 19.501 | 44.750 | 55.467 | 1.00 | 22.45 | AAAA |
| ATOM | 2089 | CA | ASP | 263 | 19.959 | 43.851 | 54.418 | 1.00 | 15.93 | AAAA |
| ATOM | 2090 | CB | ASP | 263 | 20.981 | 42.859 | 54.988 | 1.00 | 18.99 | AAAA |
| ATOM | 2091 | CG | ASP | 263 | 21.706 | 42.081 | 53.907 | 1.00 | 22.21 | AAAA |
| ATOM | 2092 | OD1 | ASP | 263 | 22.876 | 41.730 | 54.139 | 1.00 | 23.19 | AAAA |
| ATOM | 2093 | OD2 | ASP | 263 | 21.112 | 41.809 | 52.838 | 1.00 | 25.02 | AAAA |
| ATOM | 2094 | C | ASP | 263 | 18.733 | 43.165 | 53.837 | 1.00 | 22.32 | AAAA |
| ATOM | 2095 | O | ASP | 263 | 18.012 | 42.419 | 54.519 | 1.00 | 18.50 | AAAA |
| ATOM | 2096 | N | TYR | 264 | 18.500 | 43.447 | 52.564 | 1.00 | 25.21 | AAAA |
| ATOM | 2097 | CA | TYR | 264 | 17.339 | 42.936 | 51.865 | 1.00 | 29.92 | AAAA |
| ATOM | 2098 | CB | TYR | 264 | 17.077 | 43.776 | 50.596 | 1.00 | 38.48 | AAAA |
| ATOM | 2099 | CG | TYR | 264 | 17.910 | 43.431 | 49.379 | 1.00 | 54.09 | AAAA |
| ATOM | 2100 | CD1 | TYR | 264 | 17.677 | 42.249 | 48.660 | 1.00 | 69.38 | AAAA |
| ATOM | 2101 | CE1 | TYR | 264 | 18.420 | 41.930 | 47.526 | 1.00 | 68.71 | AAAA |
| ATOM | 2102 | CD2 | TYR | 264 | 18.915 | 44.286 | 48.928 | 1.00 | 66.09 | AAAA |
| ATOM | 2103 | CE2 | TYR | 264 | 19.670 | 43.975 | 47.788 | 1.00 | 74.50 | AAAA |
| ATOM | 2104 | CZ | TYR | 264 | 19.415 | 42.794 | 47.094 | 1.00 | 72.57 | AAAA |
| ATOM | 2105 | OH | TYR | 264 | 20.154 | 42.472 | 45.975 | 1.00 | 71.96 | AAAA |
| ATOM | 2106 | C | TYR | 264 | 17.445 | 41.461 | 51.532 | 1.00 | 29.55 | AAAA |
| ATOM | 2107 | O | TYR | 264 | 16.448 | 40.839 | 51.190 | 1.00 | 30.11 | AAAA |
| ATOM | 2108 | N | LEU | 265 | 18.639 | 40.891 | 51.629 | 1.00 | 24.45 | AAAA |
| ATOM | 2109 | CA | LEU | 265 | 18.753 | 39.476 | 51.337 | 1.00 | 25.36 | AAAA |
| ATOM | 2110 | CB | LEU | 265 | 20.186 | 39.089 | 50.969 | 1.00 | 29.81 | AAAA |
| ATOM | 2111 | CG | LEU | 265 | 20.509 | 39.510 | 49.531 | 1.00 | 34.43 | AAAA |
| ATOM | 2112 | CD1 | LEU | 265 | 21.847 | 38.930 | 49.100 | 1.00 | 44.38 | AAAA |

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| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2113 | CD2 | LEU | 265 | 19.422 | 38.990 | 48.603 | 1.00 | 46.72 | AAAA |
| ATOM | 2114 | C | LEU | 265 | 18.209 | 38.585 | 52.447 | 1.00 | 22.33 | AAAA |
| ATOM | 2115 | O | LEU | 265 | 18.279 | 37.364 | 52.348 | 1.00 | 23.48 | AAAA |
| ATOM | 2116 | N | SER | 266 | 17.677 | 39.194 | 53.508 | 1.00 | 17.50 | AAAA |
| ATOM | 2117 | CA | SER | 266 | 17.055 | 38.398 | 54.569 | 1.00 | 19.69 | AAAA |
| ATOM | 2118 | CB | SER | 266 | 17.912 | 38.314 | 55.845 | 1.00 | 20.73 | AAAA |
| ATOM | 2119 | OG | SER | 266 | 17.696 | 39.442 | 56.684 | 1.00 | 22.81 | AAAA |
| ATOM | 2120 | C | SER | 266 | 15.739 | 39.048 | 54.950 | 1.00 | 19.75 | AAAA |
| ATOM | 2121 | O | SER | 266 | 15.572 | 40.265 | 54.840 | 1.00 | 23.66 | AAAA |
| ATOM | 2122 | N | LYS | 267 | 14.799 | 38.229 | 55.402 | 1.00 | 18.40 | AAAA |
| ATOM | 2123 | CA | LYS | 267 | 13.527 | 38.759 | 55.851 | 1.00 | 20.64 | AAAA |
| ATOM | 2124 | CB | LYS | 267 | 12.397 | 37.787 | 55.513 | 1.00 | 20.96 | AAAA |
| ATOM | 2125 | CG | LYS | 267 | 12.269 | 37.536 | 54.025 | 1.00 | 25.60 | AAAA |
| ATOM | 2126 | CD | LYS | 267 | 12.095 | 38.823 | 53.259 | 1.00 | 33.47 | AAAA |
| ATOM | 2127 | CE | LYS | 267 | 11.985 | 38.540 | 51.772 | 1.00 | 38.49 | AAAA |
| ATOM | 2128 | NZ | LYS | 267 | 11.954 | 39.793 | 50.991 | 1.00 | 33.11 | AAAA |
| ATOM | 2129 | C | LYS | 267 | 13.601 | 38.987 | 57.365 | 1.00 | 20.63 | AAAA |
| ATOM | 2130 | O | LYS | 267 | 12.584 | 39.192 | 58.017 | 1.00 | 25.38 | AAAA |
| ATOM | 2131 | N | PHE | 268 | 14.814 | 38.937 | 57.915 | 1.00 | 18.98 | AAAA |
| ATOM | 2132 | CA | PHE | 268 | 15.034 | 39.182 | 59.345 | 1.00 | 18.50 | AAAA |
| ATOM | 2133 | CB | PHE | 268 | 16.328 | 38.510 | 59.833 | 1.00 | 20.91 | AAAA |
| ATOM | 2134 | CG | PHE | 268 | 16.252 | 37.006 | 59.967 | 1.00 | 16.96 | AAAA |
| ATOM | 2135 | CD1 | PHE | 268 | 17.374 | 36.290 | 60.415 | 1.00 | 16.61 | AAAA |
| ATOM | 2136 | CD2 | PHE | 268 | 15.081 | 36.303 | 59.682 | 1.00 | 18.13 | AAAA |
| ATOM | 2137 | CE1 | PHE | 268 | 17.331 | 34.904 | 60.581 | 1.00 | 14.81 | AAAA |
| ATOM | 2138 | CE2 | PHE | 268 | 15.027 | 34.900 | 59.849 | 1.00 | 17.45 | AAAA |
| ATOM | 2139 | CZ | PHE | 268 | 16.144 | 34.208 | 60.296 | 1.00 | 16.01 | AAAA |
| ATOM | 2140 | C | PHE | 268 | 15.179 | 40.699 | 59.510 | 1.00 | 18.33 | AAAA |
| ATOM | 2141 | O | PHE | 268 | 15.733 | 41.371 | 58.644 | 1.00 | 18.28 | AAAA |
| ATOM | 2142 | N | ASN | 269 | 14.679 | 41.236 | 60.613 | 1.00 | 21.04 | AAAA |
| ATOM | 2143 | CA | ASN | 269 | 14.763 | 42.675 | 60.859 | 1.00 | 22.89 | AAAA |
| ATOM | 2144 | CB | ASN | 269 | 13.365 | 43.298 | 60.940 | 1.00 | 20.55 | AAAA |
| ATOM | 2145 | CG | ASN | 269 | 12.551 | 43.071 | 59.686 | 1.00 | 26.13 | AAAA |
| ATOM | 2146 | OD1 | ASN | 269 | 13.060 | 43.192 | 58.571 | 1.00 | 29.17 | AAAA |
| ATOM | 2147 | ND2 | ASN | 269 | 11.268 | 42.767 | 59.860 | 1.00 | 28.26 | AAAA |
| ATOM | 2148 | C | ASN | 269 | 15.493 | 42.967 | 62.159 | 1.00 | 19.00 | AAAA |
| ATOM | 2149 | O | ASN | 269 | 14.984 | 43.683 | 63.019 | 1.00 | 21.85 | AAAA |
| ATOM | 2150 | N | LEU | 270 | 16.695 | 42.435 | 62.298 | 1.00 | 17.71 | AAAA |
| ATOM | 2151 | CA | LEU | 270 | 17.441 | 42.642 | 63.521 | 1.00 | 18.57 | AAAA |
| ATOM | 2152 | CB | LEU | 270 | 18.441 | 41.507 | 63.712 | 1.00 | 18.95 | AAAA |
| ATOM | 2153 | CG | LEU | 270 | 17.945 | 40.058 | 63.631 | 1.00 | 20.54 | AAAA |
| ATOM | 2154 | CD1 | LEU | 270 | 19.070 | 39.174 | 64.152 | 1.00 | 14.19 | AAAA |
| ATOM | 2155 | CD2 | LEU | 270 | 16.679 | 39.853 | 64.465 | 1.00 | 19.05 | AAAA |
| ATOM | 2156 | C | LEU | 270 | 18.203 | 43.971 | 63.583 | 1.00 | 19.05 | AAAA |
| ATOM | 2157 | O | LEU | 270 | 18.409 | 44.643 | 62.560 | 1.00 | 18.25 | AAAA |
| ATOM | 2158 | N | SER | 271 | 18.621 | 44.318 | 64.799 | 1.00 | 20.95 | AAAA |
| ATOM | 2159 | CA | SER | 271 | 19.414 | 45.518 | 65.081 | 1.00 | 18.28 | AAAA |
| ATOM | 2160 | CB | SER | 271 | 18.985 | 46.150 | 66.409 | 1.00 | 18.73 | AAAA |
| ATOM | 2161 | OG | SER | 271 | 19.347 | 45.327 | 67.512 | 1.00 | 22.28 | AAAA |
| ATOM | 2162 | C | SER | 271 | 20.875 | 45.073 | 65.224 | 1.00 | 19.98 | AAAA |
| ATOM | 2163 | O | SER | 271 | 21.122 | 43.899 | 65.537 | 1.00 | 18.82 | AAAA |
| ATOM | 2164 | N | ASN | 272 | 21.828 | 45.994 | 65.020 | 1.00 | 16.17 | AAAA |
| ATOM | 2165 | CA | ASN | 272 | 23.270 | 45.695 | 65.145 | 1.00 | 20.70 | AAAA |
| ATOM | 2166 | CB | ASN | 272 | 24.176 | 46.903 | 64.884 | 1.00 | 37.49 | AAAA |
| ATOM | 2167 | CG | ASN | 272 | 24.161 | 47.378 | 63.483 | 1.00 | 54.53 | AAAA |
| ATOM | 2168 | OD1 | ASN | 272 | 24.702 | 48.454 | 63.199 | 1.00 | 45.61 | AAAA |
| ATOM | 2169 | ND2 | ASN | 272 | 23.576 | 46.594 | 62.579 | 1.00 | 60.55 | AAAA |
| ATOM | 2170 | C | ASN | 272 | 23.586 | 45.343 | 66.580 | 1.00 | 18.03 | AAAA |
| ATOM | 2171 | O | ASN | 272 | 24.545 | 44.625 | 66.854 | 1.00 | 18.58 | AAAA |
| ATOM | 2172 | N | VAL | 273 | 22.831 | 45.938 | 67.500 | 1.00 | 19.57 | AAAA |
| ATOM | 2173 | CA | VAL | 273 | 23.053 | 45.698 | 68.919 | 1.00 | 22.12 | AAAA |
| ATOM | 2174 | CB | VAL | 273 | 22.345 | 46.765 | 69.765 | 1.00 | 26.91 | AAAA |
| ATOM | 2175 | CG1 | VAL | 273 | 22.440 | 46.421 | 71.233 | 1.00 | 39.69 | AAAA |
| ATOM | 2176 | CG2 | VAL | 273 | 23.034 | 48.115 | 69.531 | 1.00 | 34.73 | AAAA |
| ATOM | 2177 | C | VAL | 273 | 22.636 | 44.295 | 69.341 | 1.00 | 22.06 | AAAA |
| ATOM | 2178 | O | VAL | 273 | 23.249 | 43.708 | 70.217 | 1.00 | 16.89 | AAAA |

SUBSTITUTE SHEET (RULE 26)

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Figure 16-34

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2179 | N | ALA | 274 | 21.601 | 43.747 | 68.713 | 1.00 | 21.79 | AAAA |
| ATOM | 2180 | CA | ALA | 274 | 21.207 | 42.383 | 69.035 | 1.00 | 21.31 | AAAA |
| ATOM | 2181 | CB | ALA | 274 | 19.806 | 42.092 | 68.475 | 1.00 | 18.95 | AAAA |
| ATOM | 2182 | C | ALA | 274 | 22.259 | 41.451 | 68.400 | 1.00 | 17.83 | AAAA |
| ATOM | 2183 | O | ALA | 274 | 22.569 | 40.389 | 68.947 | 1.00 | 20.38 | AAAA |
| ATOM | 2184 | N | PHE | 275 | 22.798 | 41.859 | 67.245 | 1.00 | 16.01 | AAAA |
| ATOM | 2185 | CA | PHE | 275 | 23.828 | 41.089 | 66.536 | 1.00 | 16.46 | AAAA |
| ATOM | 2186 | CB | PHE | 275 | 24.220 | 41.835 | 65.253 | 1.00 | 24.56 | AAAA |
| ATOM | 2187 | CG | PHE | 275 | 25.363 | 41.222 | 64.492 | 1.00 | 23.01 | AAAA |
| ATOM | 2188 | CD1 | PHE | 275 | 25.209 | 40.035 | 63.788 | 1.00 | 23.88 | AAAA |
| ATOM | 2189 | CD2 | PHE | 275 | 26.590 | 41.877 | 64.443 | 1.00 | 22.40 | AAAA |
| ATOM | 2190 | CE1 | PHE | 275 | 26.266 | 39.510 | 63.038 | 1.00 | 28.74 | AAAA |
| ATOM | 2191 | CE2 | PHE | 275 | 27.654 | 41.365 | 63.700 | 1.00 | 35.03 | AAAA |
| ATOM | 2192 | CZ | PHE | 275 | 27.489 | 40.181 | 62.996 | 1.00 | 24.63 | AAAA |
| ATOM | 2193 | C | PHE | 275 | 25.030 | 40.964 | 67.469 | 1.00 | 25.06 | AAAA |
| ATOM | 2194 | O | PHE | 275 | 25.619 | 39.888 | 67.632 | 1.00 | 19.71 | AAAA |
| ATOM | 2195 | N | LEU | 276 | 25.366 | 42.080 | 68.101 | 1.00 | 17.49 | AAAA |
| ATOM | 2196 | CA | LEU | 276 | 26.482 | 42.139 | 69.030 | 1.00 | 24.23 | AAAA |
| ATOM | 2197 | CB | LEU | 276 | 26.736 | 43.606 | 69.416 | 1.00 | 20.44 | AAAA |
| ATOM | 2198 | CG | LEU | 276 | 28.001 | 43.967 | 70.211 | 1.00 | 39.65 | AAAA |
| ATOM | 2199 | CD1 | LEU | 276 | 27.948 | 45.447 | 70.589 | 1.00 | 29.65 | AAAA |
| ATOM | 2200 | CD2 | LEU | 276 | 28.102 | 43.143 | 71.460 | 1.00 | 32.41 | AAAA |
| ATOM | 2201 | C | LEU | 276 | 26.180 | 41.278 | 70.262 | 1.00 | 18.88 | AAAA |
| ATOM | 2202 | O | LEU | 276 | 27.045 | 40.529 | 70.727 | 1.00 | 17.99 | AAAA |
| ATOM | 2203 | N | LYS | 277 | 24.968 | 41.374 | 70.805 | 1.00 | 19.67 | AAAA |
| ATOM | 2204 | CA | LYS | 277 | 24.644 | 40.552 | 71.964 | 1.00 | 21.33 | AAAA |
| ATOM | 2205 | CB | LYS | 277 | 23.265 | 40.888 | 72.532 | 1.00 | 23.84 | AAAA |
| ATOM | 2206 | CG | LYS | 277 | 23.247 | 42.126 | 73.366 | 1.00 | 40.87 | AAAA |
| ATOM | 2207 | CD | LYS | 277 | 22.069 | 42.086 | 74.325 | 1.00 | 54.73 | AAAA |
| ATOM | 2208 | CE | LYS | 277 | 22.172 | 40.884 | 75.254 | 1.00 | 58.85 | AAAA |
| ATOM | 2209 | NZ | LYS | 277 | 21.051 | 40.844 | 76.228 | 1.00 | 55.34 | AAAA |
| ATOM | 2210 | C | LYS | 277 | 24.695 | 39.068 | 71.660 | 1.00 | 22.12 | AAAA |
| ATOM | 2211 | O | LYS | 277 | 25.074 | 38.264 | 72.513 | 1.00 | 22.19 | AAAA |
| ATOM | 2212 | N | ALA | 278 | 24.311 | 38.700 | 70.441 | 1.00 | 20.23 | AAAA |
| ATOM | 2213 | CA | ALA | 278 | 24.325 | 37.291 | 70.039 | 1.00 | 17.06 | AAAA |
| ATOM | 2214 | CB | ALA | 278 | 23.798 | 37.154 | 68.589 | 1.00 | 19.27 | AAAA |
| ATOM | 2215 | C | ALA | 278 | 25.760 | 36.767 | 70.127 | 1.00 | 16.94 | AAAA |
| ATOM | 2216 | O | ALA | 278 | 26.035 | 35.676 | 70.648 | 1.00 | 14.93 | AAAA |
| ATOM | 2217 | N | PHE | 279 | 26.679 | 37.564 | 69.606 | 1.00 | 18.88 | AAAA |
| ATOM | 2218 | CA | PHE | 279 | 28.099 | 37.231 | 69.626 | 1.00 | 21.01 | AAAA |
| ATOM | 2219 | CB | PHE | 279 | 28.880 | 38.392 | 68.998 | 1.00 | 16.79 | AAAA |
| ATOM | 2220 | CG | PHE | 279 | 30.370 | 38.264 | 69.120 | 1.00 | 20.23 | AAAA |
| ATOM | 2221 | CD1 | PHE | 279 | 31.062 | 37.272 | 68.423 | 1.00 | 21.61 | AAAA |
| ATOM | 2222 | CD2 | PHE | 279 | 31.088 | 39.159 | 69.905 | 1.00 | 23.24 | AAAA |
| ATOM | 2223 | CE1 | PHE | 279 | 32.461 | 37.185 | 68.509 | 1.00 | 30.98 | AAAA |
| ATOM | 2224 | CE2 | PHE | 279 | 32.480 | 39.081 | 69.995 | 1.00 | 24.82 | AAAA |
| ATOM | 2225 | CZ | PHE | 279 | 33.169 | 38.095 | 69.295 | 1.00 | 30.27 | AAAA |
| ATOM | 2226 | C | PHE | 279 | 28.576 | 36.995 | 71.067 | 1.00 | 25.48 | AAAA |
| ATOM | 2227 | O | PHE | 279 | 29.275 | 36.016 | 71.362 | 1.00 | 16.30 | AAAA |
| ATOM | 2228 | N | ASN | 280 | 28.194 | 37.898 | 71.962 | 1.00 | 22.30 | AAAA |
| ATOM | 2229 | CA | ASN | 280 | 28.599 | 37.777 | 73.352 | 1.00 | 24.49 | AAAA |
| ATOM | 2230 | CB | ASN | 280 | 28.391 | 39.109 | 74.080 | 1.00 | 27.17 | AAAA |
| ATOM | 2231 | CG | ASN | 280 | 29.344 | 40.183 | 73.578 | 1.00 | 20.88 | AAAA |
| ATOM | 2232 | OD1 | ASN | 280 | 30.503 | 39.897 | 73.273 | 1.00 | 22.95 | AAAA |
| ATOM | 2233 | ND2 | ASN | 280 | 28.875 | 41.421 | 73.522 | 1.00 | 27.85 | AAAA |
| ATOM | 2234 | C | ASN | 280 | 27.928 | 36.636 | 74.095 | 1.00 | 23.01 | AAAA |
| ATOM | 2235 | O | ASN | 280 | 28.510 | 36.062 | 75.016 | 1.00 | 21.91 | AAAA |
| ATOM | 2236 | N | ILE | 281 | 26.711 | 36.300 | 73.689 | 1.00 | 18.74 | AAAA |
| ATOM | 2237 | CA | ILE | 281 | 26.005 | 35.179 | 74.294 | 1.00 | 18.37 | AAAA |
| ATOM | 2238 | CB | ILE | 281 | 24.566 | 35.067 | 73.758 | 1.00 | 19.31 | AAAA |
| ATOM | 2239 | CG2 | ILE | 281 | 23.977 | 33.725 | 74.135 | 1.00 | 28.87 | AAAA |
| ATOM | 2240 | CG1 | ILE | 281 | 23.710 | 36.206 | 74.308 | 1.00 | 23.51 | AAAA |
| ATOM | 2241 | CD1 | ILE | 281 | 22.279 | 36.193 | 73.776 | 1.00 | 26.47 | AAAA |
| ATOM | 2242 | C | ILE | 281 | 26.743 | 33.876 | 73.965 | 1.00 | 18.54 | AAAA |
| ATOM | 2243 | O | ILE | 281 | 26.830 | 32.973 | 74.801 | 1.00 | 19.69 | AAAA |
| ATOM | 2244 | N | VAL | 282 | 27.258 | 33.765 | 72.744 | 1.00 | 17.72 | AAAA |

SUBSTITUTE SHEET (RULE 26)

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Figure 16-35

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2245 | CA | VAL | 282 | 27.976 | 32.553 | 72.352 | 1.00 | 14.89 | AAAA |
| ATOM | 2246 | CB | VAL | 282 | 28.359 | 32.565 | 70.852 | 1.00 | 18.50 | AAAA |
| ATOM | 2247 | CG1 | VAL | 282 | 29.342 | 31.440 | 70.567 | 1.00 | 20.73 | AAAA |
| ATOM | 2248 | CG2 | VAL | 282 | 27.105 | 32.363 | 69.994 | 1.00 | 17.49 | AAAA |
| ATOM | 2249 | C | VAL | 282 | 29.241 | 32.433 | 73.198 | 1.00 | 21.79 | AAAA |
| ATOM | 2250 | O | VAL | 282 | 29.568 | 31.360 | 73.715 | 1.00 | 25.80 | AAAA |
| ATOM | 2251 | N | ARG | 283 | 29.935 | 33.549 | 73.361 | 1.00 | 19.14 | AAAA |
| ATOM | 2252 | CA | ARG | 283 | 31.161 | 33.548 | 74.150 | 1.00 | 23.51 | AAAA |
| ATOM | 2253 | CB | ARG | 283 | 31.851 | 34.898 | 74.023 | 1.00 | 20.64 | AAAA |
| ATOM | 2254 | CG | ARG | 283 | 32.338 | 35.200 | 72.607 | 1.00 | 19.65 | AAAA |
| ATOM | 2255 | CD | ARG | 283 | 32.754 | 36.645 | 72.474 | 1.00 | 25.70 | AAAA |
| ATOM | 2256 | NE | ARG | 283 | 33.970 | 36.944 | 73.215 | 1.00 | 36.05 | AAAA |
| ATOM | 2257 | CZ | ARG | 283 | 34.277 | 38.147 | 73.681 | 1.00 | 34.61 | AAAA |
| ATOM | 2258 | NH1 | ARG | 283 | 33.448 | 39.169 | 73.488 | 1.00 | 35.23 | AAAA |
| ATOM | 2259 | NH2 | ARG | 283 | 35.419 | 38.332 | 74.326 | 1.00 | 29.30 | AAAA |
| ATOM | 2260 | C | ARG | 283 | 30.911 | 33.219 | 75.622 | 1.00 | 25.44 | AAAA |
| ATOM | 2261 | O | ARG | 283 | 31.754 | 32.600 | 76.272 | 1.00 | 23.12 | AAAA |
| ATOM | 2262 | N | GLU | 284 | 29.765 | 33.632 | 76.151 | 1.00 | 26.79 | AAAA |
| ATOM | 2263 | CA | GLU | 284 | 29.462 | 33.338 | 77.553 | 1.00 | 31.77 | AAAA |
| ATOM | 2264 | CB | GLU | 284 | 28.243 | 34.115 | 78.033 | 1.00 | 30.96 | AAAA |
| ATOM | 2265 | CG | GLU | 284 | 28.399 | 35.605 | 77.957 | 1.00 | 50.56 | AAAA |
| ATOM | 2266 | CD | GLU | 284 | 27.137 | 36.320 | 78.365 | 1.00 | 63.75 | AAAA |
| ATOM | 2267 | OE1 | GLU | 284 | 26.085 | 36.067 | 77.738 | 1.00 | 68.93 | AAAA |
| ATOM | 2268 | OE2 | GLU | 284 | 27.198 | 37.133 | 79.309 | 1.00 | 72.01 | AAAA |
| ATOM | 2269 | C | GLU | 284 | 29.181 | 31.862 | 77.733 | 1.00 | 31.57 | AAAA |
| ATOM | 2270 | O | GLU | 284 | 29.410 | 31.310 | 78.803 | 1.00 | 33.08 | AAAA |
| ATOM | 2271 | N | VAL | 285 | 28.673 | 31.221 | 76.686 | 1.00 | 23.37 | AAAA |
| ATOM | 2272 | CA | VAL | 285 | 28.354 | 29.807 | 76.774 | 1.00 | 23.25 | AAAA |
| ATOM | 2273 | CB | VAL | 285 | 27.221 | 29.407 | 75.789 | 1.00 | 24.77 | AAAA |
| ATOM | 2274 | CG1 | VAL | 285 | 26.952 | 27.913 | 75.881 | 1.00 | 26.98 | AAAA |
| ATOM | 2275 | CG2 | VAL | 285 | 25.940 | 30.181 | 76.107 | 1.00 | 24.98 | AAAA |
| ATOM | 2276 | C | VAL | 285 | 29.567 | 28.942 | 76.479 | 1.00 | 31.41 | AAAA |
| ATOM | 2277 | O | VAL | 285 | 29.833 | 27.983 | 77.195 | 1.00 | 25.34 | AAAA |
| ATOM | 2278 | N | PHE | 286 | 30.316 | 29.276 | 75.431 | 1.00 | 27.27 | AAAA |
| ATOM | 2279 | CA | PHE | 286 | 31.463 | 28.457 | 75.086 | 1.00 | 22.47 | AAAA |
| ATOM | 2280 | CB | PHE | 286 | 31.289 | 27.904 | 73.667 | 1.00 | 22.26 | AAAA |
| ATOM | 2281 | CG | PHE | 286 | 30.168 | 26.918 | 73.536 | 1.00 | 25.71 | AAAA |
| ATOM | 2282 | CD1 | PHE | 286 | 28.971 | 27.274 | 72.917 | 1.00 | 22.88 | AAAA |
| ATOM | 2283 | CD2 | PHE | 286 | 30.294 | 25.631 | 74.069 | 1.00 | 24.49 | AAAA |
| ATOM | 2284 | CE1 | PHE | 286 | 27.919 | 26.365 | 72.829 | 1.00 | 19.85 | AAAA |
| ATOM | 2285 | CE2 | PHE | 286 | 29.246 | 24.714 | 73.987 | 1.00 | 27.48 | AAAA |
| ATOM | 2286 | CZ | PHE | 286 | 28.056 | 25.081 | 73.367 | 1.00 | 24.59 | AAAA |
| ATOM | 2287 | C | PHE | 286 | 32.854 | 29.059 | 75.225 | 1.00 | 21.53 | AAAA |
| ATOM | 2288 | O | PHE | 286 | 33.849 | 28.417 | 74.873 | 1.00 | 27.12 | AAAA |
| ATOM | 2289 | N | GLY | 287 | 32.937 | 30.272 | 75.754 | 1.00 | 23.76 | AAAA |
| ATOM | 2290 | CA | GLY | 287 | 34.237 | 30.896 | 75.901 | 1.00 | 24.17 | AAAA |
| ATOM | 2291 | C | GLY | 287 | 34.705 | 31.419 | 74.562 | 1.00 | 27.05 | AAAA |
| ATOM | 2292 | O | GLY | 287 | 33.888 | 31.670 | 73.667 | 1.00 | 18.06 | AAAA |
| ATOM | 2293 | N | GLU | 288 | 36.017 | 31.576 | 74.414 | 1.00 | 23.21 | AAAA |
| ATOM | 2294 | CA | GLU | 288 | 36.583 | 32.085 | 73.170 | 1.00 | 24.87 | AAAA |
| ATOM | 2295 | CB | GLU | 288 | 37.968 | 32.682 | 73.410 | 1.00 | 29.25 | AAAA |
| ATOM | 2296 | CG | GLU | 288 | 37.984 | 33.933 | 74.291 | 1.00 | 42.63 | AAAA |
| ATOM | 2297 | CD | GLU | 288 | 37.114 | 35.052 | 73.745 | 1.00 | 43.77 | AAAA |
| ATOM | 2298 | OE1 | GLU | 288 | 37.235 | 35.380 | 72.544 | 1.00 | 36.82 | AAAA |
| ATOM | 2299 | OE2 | GLU | 288 | 36.317 | 35.617 | 74.521 | 1.00 | 51.56 | AAAA |
| ATOM | 2300 | C | GLU | 288 | 36.693 | 31.028 | 72.072 | 1.00 | 20.85 | AAAA |
| ATOM | 2301 | O | GLU | 288 | 36.995 | 29.856 | 72.332 | 1.00 | 18.10 | AAAA |
| ATOM | 2302 | N | GLY | 289 | 36.447 | 31.468 | 70.843 | 1.00 | 26.12 | AAAA |
| ATOM | 2303 | CA | GLY | 289 | 36.517 | 30.588 | 69.692 | 1.00 | 20.71 | AAAA |
| ATOM | 2304 | C | GLY | 289 | 37.126 | 31.318 | 68.510 | 1.00 | 18.56 | AAAA |
| ATOM | 2305 | O | GLY | 289 | 37.669 | 32.404 | 68.679 | 1.00 | 16.59 | AAAA |
| ATOM | 2306 | N | VAL | 290 | 37.032 | 30.724 | 67.322 | 1.00 | 19.86 | AAAA |
| ATOM | 2307 | CA | VAL | 290 | 37.572 | 31.312 | 66.103 | 1.00 | 19.70 | AAAA |
| ATOM | 2308 | CB | VAL | 290 | 38.150 | 30.192 | 65.184 | 1.00 | 19.04 | AAAA |
| ATOM | 2309 | CG1 | VAL | 290 | 38.667 | 30.769 | 63.853 | 1.00 | 15.54 | AAAA |
| ATOM | 2310 | CG2 | VAL | 290 | 39.296 | 29.483 | 65.920 | 1.00 | 20.40 | AAAA |

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Figure 16-36

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2311 | C | VAL | 290 | 36.408 | 32.040 | 65.427 | 1.00 | 20.90 | AAAA |
| ATOM | 2312 | O | VAL | 290 | 35.351 | 31.439 | 65.193 | 1.00 | 19.33 | AAAA |
| ATOM | 2313 | N | TYR | 291 | 36.598 | 33.325 | 65.125 | 1.00 | 15.37 | AAAA |
| ATOM | 2314 | CA | TYR | 291 | 35.543 | 34.140 | 64.524 | 1.00 | 16.79 | AAAA |
| ATOM | 2315 | CB | TYR | 291 | 35.412 | 35.438 | 65.317 | 1.00 | 16.42 | AAAA |
| ATOM | 2316 | CG | TYR | 291 | 35.375 | 35.181 | 66.808 | 1.00 | 18.60 | AAAA |
| ATOM | 2317 | CD1 | TYR | 291 | 36.366 | 35.688 | 67.659 | 1.00 | 21.77 | AAAA |
| ATOM | 2318 | CE1 | TYR | 291 | 36.368 | 35.385 | 69.030 | 1.00 | 22.55 | AAAA |
| ATOM | 2319 | CD2 | TYR | 291 | 34.388 | 34.374 | 67.361 | 1.00 | 17.34 | AAAA |
| ATOM | 2320 | CE2 | TYR | 291 | 34.381 | 34.066 | 68.718 | 1.00 | 20.24 | AAAA |
| ATOM | 2321 | CZ | TYR | 291 | 35.367 | 34.568 | 69.545 | 1.00 | 25.85 | AAAA |
| ATOM | 2322 | OH | TYR | 291 | 35.338 | 34.246 | 70.885 | 1.00 | 25.57 | AAAA |
| ATOM | 2323 | C | TYR | 291 | 35.720 | 34.446 | 63.031 | 1.00 | 14.97 | AAAA |
| ATOM | 2324 | O | TYR | 291 | 36.773 | 34.921 | 62.586 | 1.00 | 15.21 | AAAA |
| ATOM | 2325 | N | LEU | 292 | 34.660 | 34.189 | 62.273 | 1.00 | 14.06 | AAAA |
| ATOM | 2326 | CA | LEU | 292 | 34.674 | 34.392 | 60.824 | 1.00 | 15.03 | AAAA |
| ATOM | 2327 | CB | LEU | 292 | 34.461 | 33.046 | 60.108 | 1.00 | 13.66 | AAAA |
| ATOM | 2328 | CG | LEU | 292 | 35.342 | 31.856 | 60.496 | 1.00 | 19.04 | AAAA |
| ATOM | 2329 | CD1 | LEU | 292 | 34.909 | 30.615 | 59.665 | 1.00 | 15.17 | AAAA |
| ATOM | 2330 | CD2 | LEU | 292 | 36.792 | 32.190 | 60.252 | 1.00 | 19.18 | AAAA |
| ATOM | 2331 | C | LEU | 292 | 33.564 | 35.327 | 60.396 | 1.00 | 16.62 | AAAA |
| ATOM | 2332 | O | LEU | 292 | 32.575 | 35.488 | 61.107 | 1.00 | 14.76 | AAAA |
| ATOM | 2333 | N | GLY | 293 | 33.724 | 35.932 | 59.216 | 1.00 | 18.62 | AAAA |
| ATOM | 2334 | CA | GLY | 293 | 32.696 | 36.816 | 58.699 | 1.00 | 17.10 | AAAA |
| ATOM | 2335 | C | GLY | 293 | 31.611 | 35.954 | 58.068 | 1.00 | 23.44 | AAAA |
| ATOM | 2336 | O | GLY | 293 | 31.407 | 34.798 | 58.459 | 1.00 | 23.60 | AAAA |
| ATOM | 2337 | N | GLY | 294 | 30.915 | 36.501 | 57.085 | 1.00 | 24.96 | AAAA |
| ATOM | 2338 | CA | GLY | 294 | 29.871 | 35.738 | 56.434 | 1.00 | 27.07 | AAAA |
| ATOM | 2339 | C | GLY | 294 | 29.132 | 36.632 | 55.474 | 1.00 | 28.41 | AAAA |
| ATOM | 2340 | O | GLY | 294 | 29.605 | 37.722 | 55.167 | 1.00 | 25.66 | AAAA |
| ATOM | 2341 | N | GLY | 295 | 27.972 | 36.168 | 55.011 | 1.00 | 20.33 | AAAA |
| ATOM | 2342 | CA | GLY | 295 | 27.164 | 36.936 | 54.085 | 1.00 | 20.14 | AAAA |
| ATOM | 2343 | C | GLY | 295 | 26.742 | 38.244 | 54.730 | 1.00 | 25.34 | AAAA |
| ATOM | 2344 | O | GLY | 295 | 26.550 | 38.317 | 55.942 | 1.00 | 28.89 | AAAA |
| ATOM | 2345 | N | GLY | 296 | 26.614 | 39.274 | 53.909 | 1.00 | 28.52 | AAAA |
| ATOM | 2346 | CA | GLY | 296 | 26.230 | 40.598 | 54.367 | 1.00 | 23.21 | AAAA |
| ATOM | 2347 | C | GLY | 296 | 26.314 | 41.342 | 53.059 | 1.00 | 26.34 | AAAA |
| ATOM | 2348 | O | GLY | 296 | 27.359 | 41.324 | 52.414 | 1.00 | 26.05 | AAAA |
| ATOM | 2349 | N | TYR | 297 | 25.235 | 42.008 | 52.662 | 1.00 | 22.61 | AAAA |
| ATOM | 2350 | CA | TYR | 297 | 25.228 | 42.644 | 51.360 | 1.00 | 22.58 | AAAA |
| ATOM | 2351 | CB | TYR | 297 | 24.265 | 41.861 | 50.457 | 1.00 | 23.68 | AAAA |
| ATOM | 2352 | CG | TYR | 297 | 24.502 | 40.352 | 50.521 | 1.00 | 25.14 | AAAA |
| ATOM | 2353 | CD1 | TYR | 297 | 23.981 | 39.571 | 51.568 | 1.00 | 28.31 | AAAA |
| ATOM | 2354 | CE1 | TYR | 297 | 24.269 | 38.196 | 51.662 | 1.00 | 24.18 | AAAA |
| ATOM | 2355 | CD2 | TYR | 297 | 25.307 | 39.725 | 49.577 | 1.00 | 29.74 | AAAA |
| ATOM | 2356 | CE2 | TYR | 297 | 25.598 | 38.362 | 49.664 | 1.00 | 27.09 | AAAA |
| ATOM | 2357 | CZ | TYR | 297 | 25.085 | 37.606 | 50.696 | 1.00 | 28.68 | AAAA |
| ATOM | 2358 | OH | TYR | 297 | 25.407 | 36.261 | 50.739 | 1.00 | 28.17 | AAAA |
| ATOM | 2359 | C | TYR | 297 | 24.916 | 44.138 | 51.320 | 1.00 | 24.98 | AAAA |
| ATOM | 2360 | O | TYR | 297 | 24.841 | 44.714 | 50.237 | 1.00 | 26.51 | AAAA |
| ATOM | 2361 | N | HIS | 298 | 24.740 | 44.752 | 52.491 | 1.00 | 23.80 | AAAA |
| ATOM | 2362 | CA | HIS | 298 | 24.480 | 46.188 | 52.591 | 1.00 | 23.44 | AAAA |
| ATOM | 2363 | CB | HIS | 298 | 23.325 | 46.494 | 53.536 | 1.00 | 23.37 | AAAA |
| ATOM | 2364 | CG | HIS | 298 | 22.956 | 47.945 | 53.551 | 1.00 | 32.94 | AAAA |
| ATOM | 2365 | CD2 | HIS | 298 | 23.491 | 48.983 | 54.232 | 1.00 | 24.31 | AAAA |
| ATOM | 2366 | ND1 | HIS | 298 | 22.011 | 48.487 | 52.707 | 1.00 | 38.29 | AAAA |
| ATOM | 2367 | CE1 | HIS | 298 | 21.978 | 49.797 | 52.868 | 1.00 | 26.60 | AAAA |
| ATOM | 2368 | NE2 | HIS | 298 | 22.867 | 50.125 | 53.788 | 1.00 | 36.57 | AAAA |
| ATOM | 2369 | C | HIS | 298 | 25.757 | 46.775 | 53.184 | 1.00 | 23.11 | AAAA |
| ATOM | 2370 | O | HIS | 298 | 26.135 | 46.439 | 54.306 | 1.00 | 22.64 | AAAA |
| ATOM | 2371 | N | PRO | 299 | 26.430 | 47.673 | 52.445 | 1.00 | 21.07 | AAAA |
| ATOM | 2372 | CD | PRO | 299 | 26.078 | 48.207 | 51.117 | 1.00 | 27.42 | AAAA |
| ATOM | 2373 | CA | PRO | 299 | 27.676 | 48.286 | 52.910 | 1.00 | 26.62 | AAAA |
| ATOM | 2374 | CB | PRO | 299 | 28.041 | 49.228 | 51.755 | 1.00 | 28.95 | AAAA |
| ATOM | 2375 | CG | PRO | 299 | 26.678 | 49.600 | 51.196 | 1.00 | 35.16 | AAAA |
| ATOM | 2376 | C | PRO | 299 | 27.644 | 48.991 | 54.262 | 1.00 | 25.75 | AAAA |

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| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2377 | O | PRO | 299 | 28.565 | 48.845 | 55.068 | 1.00 | 24.36 | AAAA |
| ATOM | 2378 | N | TYR | 300 | 26.602 | 49.769 | 54.504 | 1.00 | 24.48 | AAAA |
| ATOM | 2379 | CA | TYR | 300 | 26.495 | 50.478 | 55.766 | 1.00 | 22.94 | AAAA |
| ATOM | 2380 | CB | TYR | 300 | 25.317 | 51.442 | 55.734 | 1.00 | 25.24 | AAAA |
| ATOM | 2381 | CG | TYR | 300 | 25.411 | 52.599 | 54.762 | 1.00 | 30.44 | AAAA |
| ATOM | 2382 | CD1 | TYR | 300 | 26.366 | 52.634 | 53.746 | 1.00 | 26.01 | AAAA |
| ATOM | 2383 | CE1 | TYR | 300 | 26.389 | 53.676 | 52.819 | 1.00 | 29.66 | AAAA |
| ATOM | 2384 | CD2 | TYR | 300 | 24.490 | 53.640 | 54.827 | 1.00 | 31.37 | AAAA |
| ATOM | 2385 | CE2 | TYR | 300 | 24.501 | 54.677 | 53.916 | 1.00 | 35.88 | AAAA |
| ATOM | 2386 | CZ | TYR | 300 | 25.448 | 54.689 | 52.913 | 1.00 | 38.44 | AAAA |
| ATOM | 2387 | OH | TYR | 300 | 25.417 | 55.700 | 51.990 | 1.00 | 33.41 | AAAA |
| ATOM | 2388 | C | TYR | 300 | 26.280 | 49.515 | 56.921 | 1.00 | 22.80 | AAAA |
| ATOM | 2389 | O | TYR | 300 | 26.895 | 49.643 | 57.983 | 1.00 | 19.14 | AAAA |
| ATOM | 2390 | N | ALA | 301 | 25.374 | 48.568 | 56.705 | 1.00 | 23.08 | AAAA |
| ATOM | 2391 | CA | ALA | 301 | 25.009 | 47.589 | 57.719 | 1.00 | 21.68 | AAAA |
| ATOM | 2392 | CB | ALA | 301 | 23.893 | 46.687 | 57.198 | 1.00 | 19.52 | AAAA |
| ATOM | 2393 | C | ALA | 301 | 26.216 | 46.762 | 58.098 | 1.00 | 23.49 | AAAA |
| ATOM | 2394 | O | ALA | 301 | 26.507 | 46.570 | 59.274 | 1.00 | 21.21 | AAAA |
| ATOM | 2395 | N | LEU | 302 | 26.904 | 46.275 | 57.072 | 1.00 | 23.19 | AAAA |
| ATOM | 2396 | CA | LEU | 302 | 28.090 | 45.463 | 57.234 | 1.00 | 20.66 | AAAA |
| ATOM | 2397 | CB | LEU | 302 | 28.602 | 45.057 | 55.844 | 1.00 | 23.31 | AAAA |
| ATOM | 2398 | CG | LEU | 302 | 29.932 | 44.335 | 55.611 | 1.00 | 36.66 | AAAA |
| ATOM | 2399 | CD1 | LEU | 302 | 29.979 | 43.849 | 54.170 | 1.00 | 38.41 | AAAA |
| ATOM | 2400 | CD2 | LEU | 302 | 31.104 | 45.255 | 55.879 | 1.00 | 28.52 | AAAA |
| ATOM | 2401 | C | LEU | 302 | 29.165 | 46.204 | 58.012 | 1.00 | 22.08 | AAAA |
| ATOM | 2402 | O | LEU | 302 | 29.653 | 45.713 | 59.020 | 1.00 | 20.43 | AAAA |
| ATOM | 2403 | N | ALA | 303 | 29.517 | 47.401 | 57.549 | 1.00 | 19.58 | AAAA |
| ATOM | 2404 | CA | ALA | 303 | 30.567 | 48.173 | 58.197 | 1.00 | 19.77 | AAAA |
| ATOM | 2405 | CB | ALA | 303 | 30.816 | 49.460 | 57.432 | 1.00 | 21.69 | AAAA |
| ATOM | 2406 | C | ALA | 303 | 30.324 | 48.485 | 59.657 | 1.00 | 19.19 | AAAA |
| ATOM | 2407 | O | ALA | 303 | 31.216 | 48.310 | 60.489 | 1.00 | 22.51 | AAAA |
| ATOM | 2408 | N | ARG | 304 | 29.128 | 48.954 | 59.993 | 1.00 | 20.12 | AAAA |
| ATOM | 2409 | CA | ARG | 304 | 28.872 | 49.296 | 61.377 | 1.00 | 18.04 | AAAA |
| ATOM | 2410 | CB | ARG | 304 | 27.566 | 50.114 | 61.511 | 1.00 | 21.09 | AAAA |
| ATOM | 2411 | CG | ARG | 304 | 27.532 | 51.481 | 60.792 | 1.00 | 24.34 | AAAA |
| ATOM | 2412 | CD | ARG | 304 | 26.259 | 52.259 | 61.206 | 1.00 | 27.09 | AAAA |
| ATOM | 2413 | NE | ARG | 304 | 25.090 | 51.398 | 61.116 | 1.00 | 45.73 | AAAA |
| ATOM | 2414 | CZ | ARG | 304 | 23.965 | 51.549 | 61.808 | 1.00 | 39.82 | AAAA |
| ATOM | 2415 | NH1 | ARG | 304 | 23.813 | 52.550 | 62.677 | 1.00 | 28.40 | AAAA |
| ATOM | 2416 | NH2 | ARG | 304 | 22.991 | 50.667 | 61.647 | 1.00 | 41.77 | AAAA |
| ATOM | 2417 | C | ARG | 304 | 28.794 | 48.073 | 62.280 | 1.00 | 21.00 | AAAA |
| ATOM | 2418 | O | ARG | 304 | 29.313 | 48.087 | 63.397 | 1.00 | 19.45 | AAAA |
| ATOM | 2419 | N | ALA | 305 | 28.159 | 47.008 | 61.796 | 1.00 | 19.93 | AAAA |
| ATOM | 2420 | CA | ALA | 305 | 28.002 | 45.809 | 62.610 | 1.00 | 18.70 | AAAA |
| ATOM | 2421 | CB | ALA | 305 | 26.998 | 44.830 | 61.933 | 1.00 | 18.26 | AAAA |
| ATOM | 2422 | C | ALA | 305 | 29.311 | 45.109 | 62.915 | 1.00 | 16.46 | AAAA |
| ATOM | 2423 | O | ALA | 306 | 29.564 | 44.736 | 64.061 | 1.00 | 19.49 | AAAA |
| ATOM | 2424 | N | TRP | 306 | 30.152 | 44.909 | 61.905 | 1.00 | 11.92 | AAAA |
| ATOM | 2425 | CA | TRP | 306 | 31.423 | 44.268 | 62.183 | 1.00 | 18.99 | AAAA |
| ATOM | 2426 | CB | TRP | 306 | 32.151 | 43.865 | 60.902 | 1.00 | 17.96 | AAAA |
| ATOM | 2427 | CG | TRP | 306 | 31.632 | 42.564 | 60.333 | 1.00 | 21.34 | AAAA |
| ATOM | 2428 | CD2 | TRP | 306 | 31.852 | 42.058 | 59.014 | 1.00 | 16.55 | AAAA |
| ATOM | 2429 | CE2 | TRP | 306 | 31.243 | 40.785 | 58.949 | 1.00 | 19.37 | AAAA |
| ATOM | 2430 | CE3 | TRP | 306 | 32.507 | 42.556 | 57.878 | 1.00 | 17.80 | AAAA |
| ATOM | 2431 | CD1 | TRP | 306 | 30.919 | 41.610 | 60.995 | 1.00 | 19.88 | AAAA |
| ATOM | 2432 | NE1 | TRP | 306 | 30.680 | 40.535 | 60.170 | 1.00 | 15.95 | AAAA |
| ATOM | 2433 | CZ2 | TRP | 306 | 31.270 | 40.002 | 57.787 | 1.00 | 24.85 | AAAA |
| ATOM | 2434 | CZ3 | TRP | 306 | 32.534 | 41.781 | 56.725 | 1.00 | 29.69 | AAAA |
| ATOM | 2435 | CH2 | TRP | 306 | 31.917 | 40.513 | 56.691 | 1.00 | 17.04 | AAAA |
| ATOM | 2436 | C | TRP | 306 | 32.289 | 45.188 | 63.018 | 1.00 | 20.26 | AAAA |
| ATOM | 2437 | O | TRP | 306 | 33.159 | 44.726 | 63.752 | 1.00 | 21.20 | AAAA |
| ATOM | 2438 | N | THR | 307 | 32.061 | 46.491 | 62.911 | 1.00 | 18.60 | AAAA |
| ATOM | 2439 | CA | THR | 307 | 32.843 | 47.412 | 63.722 | 1.00 | 16.88 | AAAA |
| ATOM | 2440 | CB | THR | 307 | 32.579 | 48.885 | 63.312 | 1.00 | 22.05 | AAAA |
| ATOM | 2441 | OG1 | THR | 307 | 33.218 | 49.132 | 62.051 | 1.00 | 21.58 | AAAA |
| ATOM | 2442 | CG2 | THR | 307 | 33.126 | 49.857 | 64.356 | 1.00 | 24.86 | AAAA |

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Figure 16-38

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2443 | C | THR | 307 | 32.493 | 47.146 | 65.187 | 1.00 | 17.47 | AAAA |
| ATOM | 2444 | O | THR | 307 | 33.377 | 47.142 | 66.039 | 1.00 | 18.94 | AAAA |
| ATOM | 2445 | N | LEU | 308 | 31.216 | 46.901 | 65.487 | 1.00 | 19.97 | AAAA |
| ATOM | 2446 | CA | LEU | 308 | 30.834 | 46.587 | 66.866 | 1.00 | 22.54 | AAAA |
| ATOM | 2447 | CB | LEU | 308 | 29.318 | 46.365 | 66.989 | 1.00 | 21.13 | AAAA |
| ATOM | 2448 | CG | LEU | 308 | 28.415 | 47.579 | 66.751 | 1.00 | 22.82 | AAAA |
| ATOM | 2449 | CD1 | LEU | 308 | 26.937 | 47.219 | 67.023 | 1.00 | 25.01 | AAAA |
| ATOM | 2450 | CD2 | LEU | 308 | 28.870 | 48.710 | 67.685 | 1.00 | 29.09 | AAAA |
| ATOM | 2451 | C | LEU | 308 | 31.578 | 45.331 | 67.336 | 1.00 | 22.98 | AAAA |
| ATOM | 2452 | O | LEU | 308 | 32.056 | 45.250 | 68.479 | 1.00 | 22.27 | AAAA |
| ATOM | 2453 | N | ILE | 309 | 31.677 | 44.342 | 66.454 | 1.00 | 22.54 | AAAA |
| ATOM | 2454 | CA | ILE | 309 | 32.377 | 43.114 | 66.801 | 1.00 | 17.09 | AAAA |
| ATOM | 2455 | CB | ILE | 309 | 32.318 | 42.073 | 65.664 | 1.00 | 18.12 | AAAA |
| ATOM | 2456 | CG2 | ILE | 309 | 33.170 | 40.870 | 66.033 | 1.00 | 24.16 | AAAA |
| ATOM | 2457 | CG1 | ILE | 309 | 30.871 | 41.655 | 65.399 | 1.00 | 18.26 | AAAA |
| ATOM | 2458 | CD1 | ILE | 309 | 30.205 | 40.989 | 66.586 | 1.00 | 26.57 | AAAA |
| ATOM | 2459 | C | ILE | 309 | 33.849 | 43.410 | 67.067 | 1.00 | 20.84 | AAAA |
| ATOM | 2460 | O | ILE | 309 | 34.426 | 42.905 | 68.031 | 1.00 | 25.20 | AAAA |
| ATOM | 2461 | N | TRP | 310 | 34.466 | 44.223 | 66.214 | 1.00 | 16.86 | AAAA |
| ATOM | 2462 | CA | TRP | 310 | 35.888 | 44.517 | 66.411 | 1.00 | 17.86 | AAAA |
| ATOM | 2463 | CB | TRP | 310 | 36.439 | 45.319 | 65.235 | 1.00 | 14.83 | AAAA |
| ATOM | 2464 | CG | TRP | 310 | 37.879 | 45.648 | 65.397 | 1.00 | 16.63 | AAAA |
| ATOM | 2465 | CD2 | TRP | 310 | 38.967 | 44.718 | 65.560 | 1.00 | 18.62 | AAAA |
| ATOM | 2466 | CE2 | TRP | 310 | 40.131 | 45.478 | 65.799 | 1.00 | 25.60 | AAAA |
| ATOM | 2467 | CE3 | TRP | 310 | 39.069 | 43.319 | 65.529 | 1.00 | 24.06 | AAAA |
| ATOM | 2468 | CD1 | TRP | 310 | 38.418 | 46.895 | 65.533 | 1.00 | 19.82 | AAAA |
| ATOM | 2469 | NE1 | TRP | 310 | 39.768 | 46.801 | 65.777 | 1.00 | 25.84 | AAAA |
| ATOM | 2470 | CZ2 | TRP | 310 | 41.383 | 44.887 | 66.006 | 1.00 | 26.14 | AAAA |
| ATOM | 2471 | CZ3 | TRP | 310 | 40.308 | 42.730 | 65.735 | 1.00 | 24.89 | AAAA |
| ATOM | 2472 | CH2 | TRP | 310 | 41.452 | 43.515 | 65.971 | 1.00 | 24.96 | AAAA |
| ATOM | 2473 | C | TRP | 310 | 36.112 | 45.263 | 67.733 | 1.00 | 20.86 | AAAA |
| ATOM | 2474 | O | TRP | 310 | 37.050 | 44.957 | 68.478 | 1.00 | 21.38 | AAAA |
| ATOM | 2475 | N | CYS | 311 | 35.242 | 46.226 | 68.030 | 1.00 | 24.22 | AAAA |
| ATOM | 2476 | CA | CYS | 311 | 35.349 | 46.971 | 69.280 | 1.00 | 27.66 | AAAA |
| ATOM | 2477 | CB | CYS | 311 | 34.297 | 48.097 | 69.343 | 1.00 | 25.37 | AAAA |
| ATOM | 2478 | SG | CYS | 311 | 34.618 | 49.528 | 68.253 | 1.00 | 27.22 | AAAA |
| ATOM | 2479 | C | CYS | 311 | 35.224 | 46.042 | 70.490 | 1.00 | 22.95 | AAAA |
| ATOM | 2480 | O | CYS | 311 | 35.986 | 46.180 | 71.441 | 1.00 | 25.47 | AAAA |
| ATOM | 2481 | N | GLU | 312 | 34.284 | 45.089 | 70.457 | 1.00 | 17.03 | AAAA |
| ATOM | 2482 | CA | GLU | 312 | 34.120 | 44.129 | 71.569 | 1.00 | 22.44 | AAAA |
| ATOM | 2483 | CB | GLU | 312 | 33.011 | 43.110 | 71.280 | 1.00 | 20.81 | AAAA |
| ATOM | 2484 | CG | GLU | 312 | 31.856 | 43.048 | 72.258 | 1.00 | 43.65 | AAAA |
| ATOM | 2485 | CD | GLU | 312 | 32.265 | 42.971 | 73.717 | 1.00 | 29.63 | AAAA |
| ATOM | 2486 | OE1 | GLU | 312 | 33.022 | 42.059 | 74.119 | 1.00 | 38.85 | AAAA |
| ATOM | 2487 | OE2 | GLU | 312 | 31.804 | 43.844 | 74.473 | 1.00 | 53.22 | AAAA |
| ATOM | 2488 | C | GLI | 312 | 35.395 | 43.309 | 71.778 | 1.00 | 27.47 | AAAA |
| ATOM | 2489 | O | GLA | 312 | 35.899 | 43.178 | 72.895 | 1.00 | 22.33 | AAAA |
| ATOM | 2490 | N | LEU | 313 | 35.899 | 42.723 | 70.696 | 1.00 | 23.82 | AAAA |
| ATOM | 2491 | CA | LEU | 313 | 37.101 | 41.889 | 70.771 | 1.00 | 20.72 | AAAA |
| ATOM | 2492 | CB | LEU | 313 | 37.380 | 41.222 | 69.422 | 1.00 | 27.82 | AAAA |
| ATOM | 2493 | CG | LEU | 313 | 36.403 | 40.167 | 68.903 | 1.00 | 33.55 | AAAA |
| ATOM | 2494 | CD1 | LEU | 313 | 36.839 | 39.738 | 67.512 | 1.00 | 24.03 | AAAA |
| ATOM | 2495 | CD2 | LEU | 313 | 36.379 | 38.981 | 69.846 | 1.00 | 28.20 | AAAA |
| ATOM | 2496 | C | LEU | 313 | 38.343 | 42.670 | 71.181 | 1.00 | 18.21 | AAAA |
| ATOM | 2497 | O | LEU | 313 | 39.119 | 42.205 | 72.017 | 1.00 | 21.48 | AAAA |
| ATOM | 2498 | N | SER | 314 | 38.492 | 43.848 | 70.580 | 1.00 | 19.41 | AAAA |
| ATOM | 2499 | CA | SER | 314 | 39.627 | 44.753 | 70.775 | 1.00 | 28.26 | AAAA |
| ATOM | 2500 | CB | SER | 314 | 39.625 | 45.821 | 69.663 | 1.00 | 22.55 | AAAA |
| ATOM | 2501 | OG | SER | 314 | 40.732 | 46.696 | 69.759 | 1.00 | 61.92 | AAAA |
| ATOM | 2502 | C | SER | 314 | 39.619 | 45.429 | 72.144 | 1.00 | 30.18 | AAAA |
| ATOM | 2503 | O | SER | 314 | 40.631 | 45.969 | 72.590 | 1.00 | 25.04 | AAAA |
| ATOM | 2504 | N | GLY | 315 | 38.477 | 45.407 | 72.806 | 1.00 | 28.04 | AAAA |
| ATOM | 2505 | CA | GLY | 315 | 38.393 | 46.009 | 74.119 | 1.00 | 33.84 | AAAA |
| ATOM | 2506 | C | GLY | 315 | 38.324 | 47.518 | 74.105 | 1.00 | 36.93 | AAAA |
| ATOM | 2507 | O | GLY | 315 | 38.811 | 48.178 | 75.022 | 1.00 | 37.00 | AAAA |
| ATOM | 2508 | N | ARG | 316 | 37.739 | 48.090 | 73.065 | 1.00 | 31.33 | AAAA |

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Figure 16-39

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2509 | CA | ARG | 316 | 37.631 | 49.536 | 73.042 | 1.00 | 39.10 | AAAA |
| ATOM | 2510 | CB | ARG | 316 | 38.347 | 50.108 | 71.830 | 1.00 | 45.15 | AAAA |
| ATOM | 2511 | CG | ARG | 316 | 37.722 | 49.834 | 70.501 | 1.00 | 46.02 | AAAA |
| ATOM | 2512 | CD | ARG | 316 | 38.620 | 50.459 | 69.449 | 1.00 | 44.83 | AAAA |
| ATOM | 2513 | NE | ARG | 316 | 39.898 | 49.767 | 69.357 | 1.00 | 37.91 | AAAA |
| ATOM | 2514 | CZ | ARG | 316 | 40.945 | 50.219 | 68.674 | 1.00 | 27.39 | AAAA |
| ATOM | 2515 | NH1 | ARG | 316 | 40.854 | 51.371 | 68.034 | 1.00 | 50.24 | AAAA |
| ATOM | 2516 | NH2 | ARG | 316 | 42.054 | 49.493 | 68.572 | 1.00 | 34.51 | AAAA |
| ATOM | 2517 | C | ARG | 316 | 36.179 | 49.984 | 73.058 | 1.00 | 35.43 | AAAA |
| ATOM | 2518 | O | ARG | 316 | 35.292 | 49.271 | 72.596 | 1.00 | 30.71 | AAAA |
| ATOM | 2519 | N | GLU | 317 | 35.931 | 51.162 | 73.612 | 1.00 | 34.06 | AAAA |
| ATOM | 2520 | CA | GLU | 317 | 34.569 | 51.663 | 73.671 | 1.00 | 37.96 | AAAA |
| ATOM | 2521 | CB | GLU | 317 | 34.481 | 52.914 | 74.552 | 1.00 | 43.60 | AAAA |
| ATOM | 2522 | CG | GLU | 317 | 33.961 | 52.630 | 75.960 | 1.00 | 60.36 | AAAA |
| ATOM | 2523 | CD | GLU | 317 | 34.768 | 51.575 | 76.701 | 1.00 | 70.70 | AAAA |
| ATOM | 2524 | OE1 | GLU | 317 | 34.375 | 51.217 | 77.832 | 1.00 | 76.71 | AAAA |
| ATOM | 2525 | OE2 | GLU | 317 | 35.793 | 51.104 | 76.162 | 1.00 | 78.36 | AAAA |
| ATOM | 2526 | C | GLU | 317 | 34.068 | 51.958 | 72.280 | 1.00 | 35.65 | AAAA |
| ATOM | 2527 | O | GLU | 317 | 34.843 | 52.322 | 71.390 | 1.00 | 32.91 | AAAA |
| ATOM | 2528 | N | VAL | 318 | 32.767 | 51.772 | 72.094 | 1.00 | 30.52 | AAAA |
| ATOM | 2529 | CA | VAL | 318 | 32.138 | 52.012 | 70.808 | 1.00 | 37.04 | AAAA |
| ATOM | 2530 | CB | VAL | 318 | 30.877 | 51.138 | 70.638 | 1.00 | 36.48 | AAAA |
| ATOM | 2531 | CG1 | VAL | 318 | 30.278 | 51.366 | 69.268 | 1.00 | 40.43 | AAAA |
| ATOM | 2532 | CG2 | VAL | 318 | 31.222 | 49.674 | 70.846 | 1.00 | 33.75 | AAAA |
| ATOM | 2533 | C | VAL | 318 | 31.719 | 53.465 | 70.737 | 1.00 | 28.96 | AAAA |
| ATOM | 2534 | O | VAL | 318 | 30.930 | 53.915 | 71.556 | 1.00 | 33.56 | AAAA |
| ATOM | 2535 | N | PRO | 319 | 32.258 | 54.229 | 69.773 | 1.00 | 29.20 | AAAA |
| ATOM | 2536 | CD | PRO | 319 | 33.243 | 53.924 | 68.726 | 1.00 | 31.62 | AAAA |
| ATOM | 2537 | CA | PRO | 319 | 31.858 | 55.637 | 69.684 | 1.00 | 28.99 | AAAA |
| ATOM | 2538 | CB | PRO | 319 | 32.709 | 56.154 | 68.528 | 1.00 | 32.17 | AAAA |
| ATOM | 2539 | CG | PRO | 319 | 32.850 | 54.926 | 67.664 | 1.00 | 41.36 | AAAA |
| ATOM | 2540 | C | PRO | 319 | 30.365 | 55.680 | 69.377 | 1.00 | 36.95 | AAAA |
| ATOM | 2541 | O | PRO | 319 | 29.847 | 54.795 | 68.695 | 1.00 | 32.86 | AAAA |
| ATOM | 2542 | N | GLU | 320 | 29.646 | 56.683 | 69.855 | 1.00 | 34.61 | AAAA |
| ATOM | 2543 | CA | GLU | 320 | 28.230 | 56.657 | 69.544 | 1.00 | 35.13 | AAAA |
| ATOM | 2544 | CB | GLU | 320 | 27.419 | 57.416 | 70.595 | 1.00 | 52.97 | AAAA |
| ATOM | 2545 | CG | GLU | 320 | 27.751 | 58.875 | 70.738 | 1.00 | 56.06 | AAAA |
| ATOM | 2546 | CD | GLU | 320 | 26.822 | 59.558 | 71.721 | 1.00 | 65.58 | AAAA |
| ATOM | 2547 | OE1 | GLU | 320 | 25.604 | 59.619 | 71.444 | 1.00 | 64.27 | AAAA |
| ATOM | 2548 | OE2 | GLU | 320 | 27.306 | 60.022 | 72.775 | 1.00 | 72.99 | AAAA |
| ATOM | 2549 | C | GLU | 320 | 27.943 | 57.192 | 68.153 | 1.00 | 35.13 | AAAA |
| ATOM | 2550 | O | GLU | 320 | 26.916 | 56.879 | 67.565 | 1.00 | 37.43 | AAAA |
| ATOM | 2551 | N | LYS | 321 | 28.880 | 57.953 | 67.604 | 1.00 | 28.22 | AAAA |
| ATOM | 2552 | CA | LYS | 321 | 28.700 | 58.555 | 66.289 | 1.00 | 36.58 | AAAA |
| ATOM | 2553 | CB | LYS | 321 | 28.666 | 60.071 | 66.454 | 1.00 | 44.87 | AAAA |
| ATOM | 2554 | CG | LYS | 321 | 29.987 | 60.606 | 67.023 | 1.00 | 55.73 | AAAA |
| ATOM | 2555 | CD | LYS | 321 | 30.305 | 60.020 | 68.410 | 1.00 | 57.27 | AAAA |
| ATOM | 2556 | CE | LYS | 321 | 31.733 | 60.310 | 68.840 | 1.00 | 54.59 | AAAA |
| ATOM | 2557 | NZ | LYS | 321 | 32.024 | 61.774 | 68.848 | 1.00 | 67.47 | AAAA |
| ATOM | 2558 | C | LYS | 321 | 29.823 | 58.211 | 65.315 | 1.00 | 34.44 | AAAA |
| ATOM | 2559 | O | LYS | 321 | 30.912 | 57.818 | 65.731 | 1.00 | 33.83 | AAAA |
| ATOM | 2560 | N | LEU | 322 | 29.549 | 58.354 | 64.019 | 1.00 | 30.21 | AAAA |
| ATOM | 2561 | CA | LEU | 322 | 30.575 | 58.135 | 62.998 | 1.00 | 29.45 | AAAA |
| ATOM | 2562 | CB | LEU | 322 | 29.966 | 57.677 | 61.677 | 1.00 | 32.21 | AAAA |
| ATOM | 2563 | CG | LEU | 322 | 29.240 | 56.338 | 61.651 | 1.00 | 38.94 | AAAA |
| ATOM | 2564 | CD1 | LEU | 322 | 29.008 | 55.977 | 60.186 | 1.00 | 38.44 | AAAA |
| ATOM | 2565 | CD2 | LEU | 322 | 30.072 | 55.261 | 62.337 | 1.00 | 42.11 | AAAA |
| ATOM | 2566 | C | LEU | 322 | 31.228 | 59.503 | 62.783 | 1.00 | 33.28 | AAAA |
| ATOM | 2567 | O | LEU | 322 | 30.544 | 60.519 | 62.872 | 1.00 | 31.45 | AAAA |
| ATOM | 2568 | N | ASN | 323 | 32.533 | 59.539 | 62.519 | 1.00 | 34.38 | AAAA |
| ATOM | 2569 | CA | ASN | 323 | 33.208 | 60.824 | 62.294 | 1.00 | 36.53 | AAAA |
| ATOM | 2570 | CB | ASN | 323 | 34.701 | 60.737 | 62.600 | 1.00 | 42.85 | AAAA |
| ATOM | 2571 | CG | ASN | 323 | 35.484 | 60.081 | 61.480 | 1.00 | 50.51 | AAAA |
| ATOM | 2572 | OD1 | ASN | 323 | 35.215 | 58.942 | 61.109 | 1.00 | 51.23 | AAAA |
| ATOM | 2573 | ND2 | ASN | 323 | 36.455 | 60.807 | 60.928 | 1.00 | 60.23 | AAAA |
| ATOM | 2574 | C | ASN | 323 | 33.027 | 61.171 | 60.822 | 1.00 | 34.69 | AAAA |

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Figure 16-40

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2575 | O | ASN | 323 | 32.429 | 60.395 | 60.075 | 1.00 | 34.06 | AAAA |
| ATOM | 2576 | N | ASN | 324 | 33.551 | 62.317 | 60.390 | 1.00 | 23.73 | AAAA |
| ATOM | 2577 | CA | ASN | 324 | 33.385 | 62.720 | 58.995 | 1.00 | 31.06 | AAAA |
| ATOM | 2578 | CB | ASN | 324 | 33.868 | 64.155 | 58.784 | 1.00 | 36.07 | AAAA |
| ATOM | 2579 | CG | ASN | 324 | 32.974 | 65.163 | 59.450 | 1.00 | 45.77 | AAAA |
| ATOM | 2580 | OD1 | ASN | 324 | 31.765 | 65.189 | 59.206 | 1.00 | 39.55 | AAAA |
| ATOM | 2581 | ND2 | ASN | 324 | 33.555 | 66.008 | 60.291 | 1.00 | 39.12 | AAAA |
| ATOM | 2582 | C | ASN | 324 | 34.047 | 61.810 | 57.971 | 1.00 | 24.87 | AAAA |
| ATOM | 2583 | O | ASN | 324 | 33.451 | 61.483 | 56.941 | 1.00 | 31.91 | AAAA |
| ATOM | 2584 | N | LYS | 325 | 35.276 | 61.405 | 58.250 | 1.00 | 27.73 | AAAA |
| ATOM | 2585 | CA | LYS | 325 | 35.991 | 60.538 | 57.333 | 1.00 | 29.55 | AAAA |
| ATOM | 2586 | CB | LYS | 325 | 37.351 | 60.182 | 57.929 | 1.00 | 37.43 | AAAA |
| ATOM | 2587 | CG | LYS | 325 | 38.250 | 59.396 | 57.004 | 1.00 | 44.84 | AAAA |
| ATOM | 2588 | CD | LYS | 325 | 39.684 | 59.435 | 57.502 | 1.00 | 50.89 | AAAA |
| ATOM | 2589 | CE | LYS | 325 | 40.191 | 60.873 | 57.561 | 1.00 | 54.82 | AAAA |
| ATOM | 2590 | NZ | LYS | 325 | 41.621 | 60.980 | 57.969 | 1.00 | 65.70 | AAAA |
| ATOM | 2591 | C | LYS | 325 | 35.161 | 59.279 | 57.078 | 1.00 | 27.99 | AAAA |
| ATOM | 2592 | O | LYS | 325 | 35.016 | 58.836 | 55.938 | 1.00 | 31.80 | AAAA |
| ATOM | 2593 | N | ALA | 326 | 34.602 | 58.721 | 58.142 | 1.00 | 26.07 | AAAA |
| ATOM | 2594 | CA | ALA | 326 | 33.781 | 57.506 | 58.030 | 1.00 | 24.38 | AAAA |
| ATOM | 2595 | CB | ALA | 326 | 33.470 | 56.982 | 59.428 | 1.00 | 27.34 | AAAA |
| ATOM | 2596 | C | ALA | 326 | 32.478 | 57.709 | 57.231 | 1.00 | 25.78 | AAAA |
| ATOM | 2597 | O | ALA | 326 | 32.131 | 56.890 | 56.369 | 1.00 | 27.37 | AAAA |
| ATOM | 2598 | N | LYS | 327 | 31.749 | 58.790 | 57.496 | 1.00 | 27.31 | AAAA |
| ATOM | 2599 | CA | LYS | 327 | 30.502 | 59.027 | 56.758 | 1.00 | 28.56 | AAAA |
| ATOM | 2600 | CB | LYS | 327 | 29.759 | 60.251 | 57.313 | 1.00 | 28.87 | AAAA |
| ATOM | 2601 | CG | LYS | 327 | 29.491 | 60.209 | 58.812 | 1.00 | 36.72 | AAAA |
| ATOM | 2602 | CD | LYS | 327 | 28.643 | 61.407 | 59.255 | 1.00 | 40.34 | AAAA |
| ATOM | 2603 | CE | LYS | 327 | 28.645 | 61.594 | 60.769 | 1.00 | 38.91 | AAAA |
| ATOM | 2604 | NZ | LYS | 327 | 28.163 | 60.429 | 61.556 | 1.00 | 47.67 | AAAA |
| ATOM | 2605 | C | LYS | 327 | 30.792 | 59.244 | 55.269 | 1.00 | 29.15 | AAAA |
| ATOM | 2606 | O | LYS | 327 | 30.097 | 58.719 | 54.393 | 1.00 | 27.76 | AAAA |
| ATOM | 2607 | N | GLU | 328 | 31.829 | 60.015 | 54.972 | 1.00 | 31.59 | AAAA |
| ATOM | 2608 | CA | GLU | 328 | 32.167 | 60.265 | 53.581 | 1.00 | 28.93 | AAAA |
| ATOM | 2609 | CB | GLU | 328 | 33.257 | 61.332 | 53.515 | 1.00 | 32.30 | AAAA |
| ATOM | 2610 | CG | GLU | 328 | 32.745 | 62.652 | 54.067 | 1.00 | 47.50 | AAAA |
| ATOM | 2611 | CD | GLU | 328 | 33.764 | 63.772 | 54.032 | 1.00 | 46.67 | AAAA |
| ATOM | 2612 | OE1 | GLU | 328 | 34.325 | 64.037 | 52.951 | 1.00 | 56.88 | AAAA |
| ATOM | 2613 | OE2 | GLU | 328 | 33.984 | 64.402 | 55.087 | 1.00 | 42.24 | AAAA |
| ATOM | 2614 | C | GLU | 328 | 32.575 | 58.975 | 52.871 | 1.00 | 30.46 | AAAA |
| ATOM | 2615 | O | GLU | 328 | 32.226 | 58.753 | 51.704 | 1.00 | 26.29 | AAAA |
| ATOM | 2616 | N | LEU | 329 | 33.292 | 58.112 | 53.584 | 1.00 | 24.93 | AAAA |
| ATOM | 2617 | CA | LEU | 329 | 33.701 | 56.828 | 53.017 | 1.00 | 24.80 | AAAA |
| ATOM | 2618 | CB | LEU | 329 | 34.478 | 56.003 | 54.053 | 1.00 | 25.70 | AAAA |
| ATOM | 2619 | CG | LEU | 329 | 34.730 | 54.522 | 53.703 | 1.00 | 19.71 | AAAA |
| ATOM | 2620 | CD1 | LEU | 329 | 35.569 | 54.413 | 52.430 | 1.00 | 25.26 | AAAA |
| ATOM | 2621 | CD2 | LEU | 329 | 35.412 | 53.833 | 54.863 | 1.00 | 24.73 | AAAA |
| ATOM | 2622 | C | LEU | 329 | 32.443 | 56.059 | 52.603 | 1.00 | 23.50 | AAAA |
| ATOM | 2623 | O | LEU | 329 | 32.310 | 55.650 | 51.453 | 1.00 | 25.60 | AAAA |
| ATOM | 2624 | N | LEU | 330 | 31.516 | 55.881 | 53.539 | 1.00 | 23.02 | AAAA |
| ATOM | 2625 | CA | LEU | 330 | 30.289 | 55.145 | 53.242 | 1.00 | 23.85 | AAAA |
| ATOM | 2626 | CB | LEU | 330 | 29.414 | 55.030 | 54.484 | 1.00 | 21.74 | AAAA |
| ATOM | 2627 | CG | LEU | 330 | 30.039 | 54.252 | 55.642 | 1.00 | 25.29 | AAAA |
| ATOM | 2628 | CD1 | LEU | 330 | 28.984 | 54.053 | 56.724 | 1.00 | 30.58 | AAAA |
| ATOM | 2629 | CD2 | LEU | 330 | 30.538 | 52.905 | 55.168 | 1.00 | 22.44 | AAAA |
| ATOM | 2630 | C | LEU | 330 | 29.491 | 55.769 | 52.113 | 1.00 | 26.94 | AAAA |
| ATOM | 2631 | O | LEU | 330 | 28.968 | 55.060 | 51.252 | 1.00 | 26.65 | AAAA |
| ATOM | 2632 | N | LYS | 331 | 29.404 | 57.097 | 52.111 | 1.00 | 30.82 | AAAA |
| ATOM | 2633 | CA | LYS | 331 | 28.667 | 57.795 | 51.066 | 1.00 | 29.53 | AAAA |
| ATOM | 2634 | CB | LYS | 331 | 28.537 | 59.292 | 51.407 | 1.00 | 29.67 | AAAA |
| ATOM | 2635 | CG | LYS | 331 | 27.814 | 59.567 | 52.714 | 1.00 | 36.06 | AAAA |
| ATOM | 2636 | CD | LYS | 331 | 27.688 | 61.055 | 52.990 | 1.00 | 42.75 | AAAA |
| ATOM | 2637 | CE | LYS | 331 | 26.828 | 61.737 | 51.939 | 1.00 | 53.98 | AAAA |
| ATOM | 2638 | NZ | LYS | 331 | 26.634 | 63.185 | 52.234 | 1.00 | 67.57 | AAAA |
| ATOM | 2639 | C | LYS | 331 | 29.315 | 57.628 | 49.692 | 1.00 | 30.07 | AAAA |
| ATOM | 2640 | O | LYS | 331 | 28.634 | 57.759 | 48.672 | 1.00 | 36.20 | AAAA |

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Figure 16-41

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2641 | N | SER | 332 | 30.608 | 57.305 | 49.657 | 1.00 | 30.08 | AAAA |
| ATOM | 2642 | CA | SER | 332 | 31.322 | 57.153 | 48.385 | 1.00 | 33.35 | AAAA |
| ATOM | 2643 | CB | SER | 332 | 32.834 | 57.312 | 48.590 | 1.00 | 40.36 | AAAA |
| ATOM | 2644 | OG | SER | 332 | 33.396 | 56.169 | 49.219 | 1.00 | 34.04 | AAAA |
| ATOM | 2645 | C | SER | 332 | 31.061 | 55.821 | 47.693 | 1.00 | 37.72 | AAAA |
| ATOM | 2646 | O | SER | 332 | 31.354 | 55.661 | 46.507 | 1.00 | 30.78 | AAAA |
| ATOM | 2647 | N | ILE | 333 | 30.521 | 54.865 | 48.440 | 1.00 | 30.61 | AAAA |
| ATOM | 2648 | CA | ILE | 333 | 30.219 | 53.547 | 47.899 | 1.00 | 37.59 | AAAA |
| ATOM | 2649 | CB | ILE | 333 | 29.901 | 52.551 | 49.022 | 1.00 | 33.59 | AAAA |
| ATOM | 2650 | CG2 | ILE | 333 | 29.738 | 51.146 | 48.442 | 1.00 | 37.05 | AAAA |
| ATOM | 2651 | CG1 | ILE | 333 | 31.015 | 52.564 | 50.065 | 1.00 | 38.95 | AAAA |
| ATOM | 2652 | CD1 | ILE | 333 | 30.706 | 51.727 | 51.282 | 1.00 | 46.83 | AAAA |
| ATOM | 2653 | C | ILE | 333 | 28.990 | 53.620 | 46.998 | 1.00 | 43.41 | AAAA |
| ATOM | 2654 | O | ILE | 333 | 27.889 | 53.876 | 47.479 | 1.00 | 46.24 | AAAA |
| ATOM | 2655 | N | ASP | 334 | 29.158 | 53.423 | 45.696 | 1.00 | 47.97 | AAAA |
| ATOM | 2656 | CA | ASP | 334 | 27.976 | 53.447 | 44.847 | 1.00 | 53.47 | AAAA |
| ATOM | 2657 | CB | ASP | 334 | 28.333 | 53.535 | 43.358 | 1.00 | 61.52 | AAAA |
| ATOM | 2658 | CG | ASP | 334 | 29.223 | 52.406 | 42.897 | 1.00 | 64.75 | AAAA |
| ATOM | 2659 | OD1 | ASP | 334 | 29.379 | 52.248 | 41.666 | 1.00 | 66.93 | AAAA |
| ATOM | 2660 | OD2 | ASP | 334 | 29.779 | 51.691 | 43.758 | 1.00 | 65.93 | AAAA |
| ATOM | 2661 | C | ASP | 334 | 27.248 | 52.144 | 45.161 | 1.00 | 51.83 | AAAA |
| ATOM | 2662 | O | ASP | 334 | 27.626 | 51.067 | 44.699 | 1.00 | 46.80 | AAAA |
| ATOM | 2663 | N | PHE | 335 | 26.215 | 52.249 | 45.986 | 1.00 | 54.96 | AAAA |
| ATOM | 2664 | CA | PHE | 335 | 25.455 | 51.080 | 46.392 | 1.00 | 50.60 | AAAA |
| ATOM | 2665 | CB | PHE | 335 | 25.413 | 51.003 | 47.920 | 1.00 | 39.55 | AAAA |
| ATOM | 2666 | CG | PHE | 335 | 24.380 | 50.054 | 48.440 | 1.00 | 37.98 | AAAA |
| ATOM | 2667 | CD1 | PHE | 335 | 24.389 | 48.715 | 48.054 | 1.00 | 46.72 | AAAA |
| ATOM | 2668 | CD2 | PHE | 335 | 23.362 | 50.506 | 49.262 | 1.00 | 34.23 | AAAA |
| ATOM | 2669 | CE1 | PHE | 335 | 23.389 | 47.842 | 48.478 | 1.00 | 49.80 | AAAA |
| ATOM | 2670 | CE2 | PHE | 335 | 22.361 | 49.644 | 49.689 | 1.00 | 48.51 | AAAA |
| ATOM | 2671 | CZ | PHE | 335 | 22.373 | 48.309 | 49.296 | 1.00 | 40.44 | AAAA |
| ATOM | 2672 | C | PHE | 335 | 24.033 | 51.000 | 45.839 | 1.00 | 54.52 | AAAA |
| ATOM | 2673 | O | PHE | 335 | 23.603 | 49.939 | 45.379 | 1.00 | 59.24 | AAAA |
| ATOM | 2674 | N | GLU | 336 | 23.302 | 52.108 | 45.888 | 1.00 | 50.94 | AAAA |
| ATOM | 2675 | CA | GLU | 336 | 21.923 | 52.119 | 45.406 | 1.00 | 57.05 | AAAA |
| ATOM | 2676 | CB | GLU | 336 | 21.853 | 51.751 | 43.924 | 1.00 | 60.27 | AAAA |
| ATOM | 2677 | CG | GLU | 336 | 20.430 | 51.627 | 43.422 | 1.00 | 68.55 | AAAA |
| ATOM | 2678 | CD | GLU | 336 | 20.352 | 51.126 | 42.001 | 1.00 | 80.03 | AAAA |
| ATOM | 2679 | OE1 | GLU | 336 | 20.860 | 50.013 | 41.735 | 1.00 | 84.64 | AAAA |
| ATOM | 2680 | OE2 | GLU | 336 | 19.777 | 51.841 | 41.153 | 1.00 | 80.68 | AAAA |
| ATOM | 2681 | C | GLU | 336 | 21.065 | 51.135 | 46.201 | 1.00 | 55.73 | AAAA |
| ATOM | 2682 | O | GLU | 336 | 21.219 | 49.917 | 46.089 | 1.00 | 51.33 | AAAA |
| ATOM | 2683 | N | GLU | 337 | 20.151 | 51.679 | 46.992 | 1.00 | 49.54 | AAAA |
| ATOM | 2684 | CA | GLU | 337 | 19.267 | 50.880 | 47.821 | 1.00 | 48.19 | AAAA |
| ATOM | 2685 | CB | GLU | 337 | 18.510 | 51.822 | 48.764 | 1.00 | 47.73 | AAAA |
| ATOM | 2686 | CG | GLU | 337 | 18.084 | 51.205 | 50.077 | 1.00 | 55.69 | AAAA |
| ATOM | 2687 | CD | GLU | 337 | 19.269 | 50.720 | 50.904 | 1.00 | 50.17 | AAAA |
| ATOM | 2688 | OE1 | GLU | 337 | 20.111 | 51.548 | 51.345 | 1.00 | 36.03 | AAAA |
| ATOM | 2689 | OE2 | GLU | 337 | 19.358 | 49.494 | 51.105 | 1.00 | 51.25 | AAAA |
| ATOM | 2690 | C | GLU | 337 | 18.294 | 50.083 | 46.936 | 1.00 | 49.13 | AAAA |
| ATOM | 2691 | O | GLU | 337 | 17.816 | 50.588 | 45.916 | 1.00 | 48.61 | AAAA |
| ATOM | 2692 | N | PHE | 338 | 18.015 | 48.837 | 47.313 | 1.00 | 48.15 | AAAA |
| ATOM | 2693 | CA | PHE | 338 | 17.092 | 48.000 | 46.547 | 1.00 | 48.12 | AAAA |
| ATOM | 2694 | CB | PHE | 338 | 16.870 | 46.658 | 47.249 | 1.00 | 54.54 | AAAA |
| ATOM | 2695 | CG | PHE | 338 | 15.883 | 45.777 | 46.548 | 1.00 | 57.22 | AAAA |
| ATOM | 2696 | CD1 | PHE | 338 | 16.115 | 45.366 | 45.243 | 1.00 | 60.01 | AAAA |
| ATOM | 2697 | CD2 | PHE | 338 | 14.699 | 45.398 | 47.171 | 1.00 | 55.04 | AAAA |
| ATOM | 2698 | CE1 | PHE | 338 | 15.185 | 44.597 | 44.566 | 1.00 | 60.84 | AAAA |
| ATOM | 2699 | CE2 | PHE | 338 | 13.758 | 44.624 | 46.497 | 1.00 | 59.41 | AAAA |
| ATOM | 2700 | CZ | PHE | 338 | 14.002 | 44.224 | 45.189 | 1.00 | 57.18 | AAAA |
| ATOM | 2701 | C | PHE | 338 | 15.755 | 48.714 | 46.380 | 1.00 | 45.46 | AAAA |
| ATOM | 2702 | O | PHE | 338 | 15.274 | 48.900 | 45.263 | 1.00 | 51.11 | AAAA |
| ATOM | 2703 | N | ASP | 339 | 15.154 | 49.098 | 47.501 | 1.00 | 40.38 | AAAA |
| ATOM | 2704 | CA | ASP | 339 | 13.890 | 49.820 | 47.488 | 1.00 | 49.97 | AAAA |
| ATOM | 2705 | CB | ASP | 339 | 13.270 | 49.821 | 48.886 | 1.00 | 53.23 | AAAA |
| ATOM | 2706 | CG | ASP | 339 | 12.000 | 50.659 | 48.968 | 1.00 | 57.40 | AAAA |

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Figure 16-42

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2707 | OD1 | ASP | 339 | 12.039 | 51.858 | 48.616 | 1.00 | 53.79 | AAAA |
| ATOM | 2708 | OD2 | ASP | 339 | 10.963 | 50.118 | 49.401 | 1.00 | 51.15 | AAAA |
| ATOM | 2709 | C | ASP | 339 | 14.215 | 51.248 | 47.076 | 1.00 | 55.06 | AAAA |
| ATOM | 2710 | O | ASP | 339 | 14.994 | 51.922 | 47.748 | 1.00 | 56.47 | AAAA |
| ATOM | 2711 | N | ASP | 340 | 13.623 | 51.708 | 45.978 | 1.00 | 58.46 | AAAA |
| ATOM | 2712 | CA | ASP | 340 | 13.874 | 53.059 | 45.484 | 1.00 | 67.72 | AAAA |
| ATOM | 2713 | CB | ASP | 340 | 12.683 | 53.559 | 44.664 | 1.00 | 71.52 | AAAA |
| ATOM | 2714 | CG | ASP | 340 | 12.611 | 52.913 | 43.295 | 1.00 | 79.72 | AAAA |
| ATOM | 2715 | OD1 | ASP | 340 | 12.528 | 51.667 | 43.224 | 1.00 | 86.74 | AAAA |
| ATOM | 2716 | OD2 | ASP | 340 | 12.640 | 53.655 | 42.288 | 1.00 | 83.40 | AAAA |
| ATOM | 2717 | C | ASP | 340 | 14.209 | 54.072 | 46.572 | 1.00 | 69.65 | AAAA |
| ATOM | 2718 | O | ASP | 340 | 15.204 | 54.794 | 46.463 | 1.00 | 70.13 | AAAA |
| ATOM | 2719 | N | GLU | 341 | 13.392 | 54.130 | 47.620 | 1.00 | 67.11 | AAAA |
| ATOM | 2720 | CA | GLU | 341 | 13.668 | 55.077 | 48.689 | 1.00 | 67.87 | AAAA |
| ATOM | 2721 | CB | GLU | 341 | 13.195 | 56.478 | 48.278 | 1.00 | 74.87 | AAAA |
| ATOM | 2722 | CG | GLU | 341 | 13.502 | 57.576 | 49.298 | 1.00 | 82.72 | AAAA |
| ATOM | 2723 | CD | GLU | 341 | 13.162 | 58.974 | 48.790 | 1.00 | 90.80 | AAAA |
| ATOM | 2724 | OE1 | GLU | 341 | 11.988 | 59.215 | 48.431 | 1.00 | 90.38 | AAAA |
| ATOM | 2725 | OE2 | GLU | 341 | 14.072 | 59.835 | 48.752 | 1.00 | 93.36 | AAAA |
| ATOM | 2726 | C | GLU | 341 | 13.101 | 54.719 | 50.058 | 1.00 | 60.22 | AAAA |
| ATOM | 2727 | O | GLU | 341 | 11.929 | 54.955 | 50.347 | 1.00 | 58.81 | AAAA |
| ATOM | 2728 | N | VAL | 342 | 13.956 | 54.144 | 50.897 | 1.00 | 57.28 | AAAA |
| ATOM | 2729 | CA | VAL | 342 | 13.594 | 53.781 | 52.262 | 1.00 | 52.09 | AAAA |
| ATOM | 2730 | CB | VAL | 342 | 14.195 | 52.419 | 52.669 | 1.00 | 53.17 | AAAA |
| ATOM | 2731 | CG1 | VAL | 342 | 13.730 | 52.042 | 54.070 | 1.00 | 46.16 | AAAA |
| ATOM | 2732 | CG2 | VAL | 342 | 13.815 | 51.356 | 51.663 | 1.00 | 59.09 | AAAA |
| ATOM | 2733 | C | VAL | 342 | 14.263 | 54.843 | 53.124 | 1.00 | 53.31 | AAAA |
| ATOM | 2734 | O | VAL | 342 | 13.763 | 55.230 | 54.185 | 1.00 | 57.79 | AAAA |
| ATOM | 2735 | N | ASP | 343 | 15.398 | 55.306 | 52.610 | 1.00 | 46.24 | AAAA |
| ATOM | 2736 | CA | ASP | 343 | 16.268 | 56.289 | 53.243 | 1.00 | 42.60 | AAAA |
| ATOM | 2737 | CB | ASP | 343 | 15.521 | 57.510 | 53.781 | 1.00 | 43.88 | AAAA |
| ATOM | 2738 | CG | ASP | 343 | 16.480 | 58.581 | 54.290 | 1.00 | 46.82 | AAAA |
| ATOM | 2739 | OD1 | ASP | 343 | 16.028 | 59.581 | 54.887 | 1.00 | 46.16 | AAAA |
| ATOM | 2740 | OD2 | ASP | 343 | 17.700 | 58.414 | 54.075 | 1.00 | 33.01 | AAAA |
| ATOM | 2741 | C | ASP | 343 | 17.012 | 55.636 | 54.395 | 1.00 | 35.45 | AAAA |
| ATOM | 2742 | O | ASP | 343 | 16.487 | 55.480 | 55.502 | 1.00 | 29.39 | AAAA |
| ATOM | 2743 | N | ARG | 344 | 18.247 | 55.249 | 54.124 | 1.00 | 30.51 | AAAA |
| ATOM | 2744 | CA | ARG | 344 | 19.059 | 54.613 | 55.140 | 1.00 | 29.43 | AAAA |
| ATOM | 2745 | CB | ARG | 344 | 19.736 | 53.377 | 54.561 | 1.00 | 30.10 | AAAA |
| ATOM | 2746 | CG | ARG | 344 | 18.803 | 52.258 | 54.180 | 1.00 | 33.95 | AAAA |
| ATOM | 2747 | CD | ARG | 344 | 17.981 | 51.770 | 55.365 | 1.00 | 20.92 | AAAA |
| ATOM | 2748 | NE | ARG | 344 | 17.120 | 50.673 | 54.936 | 1.00 | 29.72 | AAAA |
| ATOM | 2749 | CZ | ARG | 344 | 16.110 | 50.176 | 55.639 | 1.00 | 29.13 | AAAA |
| ATOM | 2750 | NH1 | ARG | 344 | 15.805 | 50.668 | 56.835 | 1.00 | 29.63 | AAAA |
| ATOM | 2751 | NH2 | ARG | 344 | 15.379 | 49.198 | 55.120 | 1.00 | 27.19 | AAAA |
| ATOM | 2752 | C | ARG | 344 | 20.116 | 55.69 | 55.660 | 1.00 | 34.31 | AAAA |
| ATOM | 2753 | O | ARG | 344 | 21.005 | 55.57 | 56.391 | 1.00 | 29.09 | AAAA |
| ATOM | 2754 | N | SER | 345 | 20.011 | 56.45 | 55.294 | 1.00 | 28.34 | AAAA |
| ATOM | 2755 | CA | SER | 345 | 20.999 | 57.839 | 55.715 | 1.00 | 30.95 | AAAA |
| ATOM | 2756 | CB | SER | 345 | 20.669 | 59.199 | 55.109 | 1.00 | 29.56 | AAAA |
| ATOM | 2757 | OG | SER | 345 | 19.429 | 59.648 | 55.610 | 1.00 | 29.38 | AAAA |
| ATOM | 2758 | C | SER | 345 | 21.137 | 57.988 | 57.230 | 1.00 | 30.92 | AAAA |
| ATOM | 2759 | O | SER | 345 | 22.155 | 58.488 | 57.718 | 1.00 | 31.15 | AAAA |
| ATOM | 2760 | N | TYR | 346 | 20.116 | 57.576 | 57.975 | 1.00 | 25.64 | AAAA |
| ATOM | 2761 | CA | TYR | 346 | 20.158 | 57.659 | 59.433 | 1.00 | 26.81 | AAAA |
| ATOM | 2762 | CB | TYR | 346 | 18.823 | 57.189 | 60.006 | 1.00 | 34.41 | AAAA |
| ATOM | 2763 | CG | TYR | 346 | 18.529 | 55.723 | 59.716 | 1.00 | 27.35 | AAAA |
| ATOM | 2764 | CD1 | TYR | 346 | 19.003 | 54.708 | 60.556 | 1.00 | 24.87 | AAAA |
| ATOM | 2765 | CE1 | TYR | 346 | 18.744 | 53.352 | 60.278 | 1.00 | 28.05 | AAAA |
| ATOM | 2766 | CD2 | TYR | 346 | 17.795 | 55.358 | 58.588 | 1.00 | 27.70 | AAAA |
| ATOM | 2767 | CE2 | TYR | 346 | 17.533 | 54.008 | 58.297 | 1.00 | 26.59 | AAAA |
| ATOM | 2768 | CZ | TYR | 346 | 18.008 | 53.015 | 59.145 | 1.00 | 33.75 | AAAA |
| ATOM | 2769 | OH | TYR | 346 | 17.737 | 51.691 | 58.855 | 1.00 | 26.06 | AAAA |
| ATOM | 2770 | C | TYR | 346 | 21.277 | 56.766 | 59.977 | 1.00 | 25.57 | AAAA |
| ATOM | 2771 | O | TYR | 346 | 21.769 | 56.970 | 61.085 | 1.00 | 28.07 | AAAA |
| ATOM | 2772 | N | MET | 347 | 21.666 | 55.761 | 59.198 | 1.00 | 29.08 | AAAA |

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Figure 16-43

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2773 | CA | MET | 347 | 22.720 | 54.837 | 59.622 | 1.00 | 24.19 | AAAA |
| ATOM | 2774 | CB | MET | 347 | 22.844 | 53.678 | 58.628 | 1.00 | 24.87 | AAAA |
| ATOM | 2775 | CG | MET | 347 | 21.609 | 52.806 | 58.543 | 1.00 | 23.66 | AAAA |
| ATOM | 2776 | SD | MET | 347 | 21.780 | 51.503 | 57.267 | 1.00 | 27.02 | AAAA |
| ATOM | 2777 | CE | MET | 347 | 22.115 | 52.375 | 55.896 | 1.00 | 37.69 | AAAA |
| ATOM | 2778 | C | MET | 347 | 24.054 | 55.540 | 59.737 | 1.00 | 29.45 | AAAA |
| ATOM | 2779 | O | MET | 347 | 24.937 | 55.092 | 60.479 | 1.00 | 28.08 | AAAA |
| ATOM | 2780 | N | LEU | 348 | 24.188 | 56.650 | 59.007 | 1.00 | 23.71 | AAAA |
| ATOM | 2781 | CA | LEU | 348 | 25.418 | 57.446 | 58.998 | 1.00 | 34.11 | AAAA |
| ATOM | 2782 | CB | LEU | 348 | 25.463 | 58.351 | 57.757 | 1.00 | 25.37 | AAAA |
| ATOM | 2783 | CG | LEU | 348 | 25.320 | 57.785 | 56.344 | 1.00 | 30.38 | AAAA |
| ATOM | 2784 | CD1 | LEU | 348 | 25.307 | 58.944 | 55.340 | 1.00 | 27.44 | AAAA |
| ATOM | 2785 | CD2 | LEU | 348 | 26.459 | 56.814 | 56.041 | 1.00 | 36.44 | AAAA |
| ATOM | 2786 | C | LEU | 348 | 25.507 | 58.332 | 60.237 | 1.00 | 36.09 | AAAA |
| ATOM | 2787 | O | LEU | 348 | 26.561 | 58.894 | 60.539 | 1.00 | 33.30 | AAAA |
| ATOM | 2788 | N | GLU | 349 | 24.394 | 58.445 | 60.953 | 1.00 | 30.51 | AAAA |
| ATOM | 2789 | CA | GLU | 349 | 24.313 | 59.292 | 62.136 | 1.00 | 35.53 | AAAA |
| ATOM | 2790 | CB | GLU | 349 | 22.908 | 59.896 | 62.217 | 1.00 | 31.35 | AAAA |
| ATOM | 2791 | CG | GLU | 349 | 22.518 | 60.717 | 61.006 | 1.00 | 29.09 | AAAA |
| ATOM | 2792 | CD | GLU | 349 | 23.481 | 61.859 | 60.746 | 1.00 | 31.78 | AAAA |
| ATOM | 2793 | OE1 | GLU | 349 | 23.937 | 62.476 | 61.730 | 1.00 | 30.98 | AAAA |
| ATOM | 2794 | OE2 | GLU | 349 | 23.766 | 62.155 | 59.569 | 1.00 | 30.67 | AAAA |
| ATOM | 2795 | C | GLU | 349 | 24.663 | 58.633 | 63.471 | 1.00 | 38.48 | AAAA |
| ATOM | 2796 | O | GLU | 349 | 24.727 | 59.303 | 64.502 | 1.00 | 40.12 | AAAA |
| ATOM | 2797 | N | THR | 350 | 24.878 | 57.326 | 63.461 | 1.00 | 33.58 | AAAA |
| ATOM | 2798 | CA | THR | 350 | 25.221 | 56.612 | 64.681 | 1.00 | 29.74 | AAAA |
| ATOM | 2799 | CB | THR | 350 | 23.992 | 56.363 | 65.559 | 1.00 | 35.91 | AAAA |
| ATOM | 2800 | OG1 | THR | 350 | 23.421 | 57.615 | 65.952 | 1.00 | 45.03 | AAAA |
| ATOM | 2801 | CG2 | THR | 350 | 24.382 | 55.586 | 66.806 | 1.00 | 49.48 | AAAA |
| ATOM | 2802 | C | THR | 350 | 25.821 | 55.267 | 64.330 | 1.00 | 30.63 | AAAA |
| ATOM | 2803 | O | THR | 350 | 25.535 | 54.709 | 63.274 | 1.00 | 26.62 | AAAA |
| ATOM | 2804 | N | LEU | 351 | 26.644 | 54.740 | 65.225 | 1.00 | 29.07 | AAAA |
| ATOM | 2805 | CA | LEU | 351 | 27.271 | 53.461 | 64.972 | 1.00 | 24.59 | AAAA |
| ATOM | 2806 | CB | LEU | 351 | 28.584 | 53.367 | 65.757 | 1.00 | 29.91 | AAAA |
| ATOM | 2807 | CG | LEU | 351 | 29.591 | 52.327 | 65.267 | 1.00 | 39.62 | AAAA |
| ATOM | 2808 | CD1 | LEU | 351 | 30.887 | 52.467 | 66.039 | 1.00 | 37.09 | AAAA |
| ATOM | 2809 | CD2 | LEU | 351 | 29.024 | 50.935 | 65.415 | 1.00 | 54.03 | AAAA |
| ATOM | 2810 | C | LEU | 351 | 26.314 | 52.336 | 65.377 | 1.00 | 29.71 | AAAA |
| ATOM | 2811 | O | LEU | 351 | 26.130 | 51.364 | 64.641 | 1.00 | 30.53 | AAAA |
| ATOM | 2812 | N | LYS | 352 | 25.697 | 52.481 | 66.543 | 1.00 | 28.64 | AAAA |
| ATOM | 2813 | CA | LYS | 352 | 24.763 | 51.479 | 67.061 | 1.00 | 32.72 | AAAA |
| ATOM | 2814 | CB | LYS | 352 | 24.913 | 51.381 | 68.581 | 1.00 | 27.37 | AAAA |
| ATOM | 2815 | CG | LYS | 352 | 26.230 | 50.787 | 69.034 | 1.00 | 43.48 | AAAA |
| ATOM | 2816 | CD | LYS | 352 | 26.536 | 51.068 | 70.504 | 1.00 | 46.77 | AAAA |
| ATOM | 2817 | CE | LYS | 352 | 25.484 | 50.538 | 71.451 | 1.00 | 51.52 | AAAA |
| ATOM | 2818 | NZ | LYS | 352 | 25.850 | 50.859 | 72.866 | 1.00 | 62.08 | AAAA |
| ATOM | 2819 | C | LYS | 352 | 23.330 | 51.856 | 66.731 | 1.00 | 32.49 | AAAA |
| ATOM | 2820 | O | LYS | 352 | 22.953 | 53.010 | 66.882 | 1.00 | 31.90 | AAAA |
| ATOM | 2821 | N | ASP | 353 | 22.525 | 50.916 | 66.244 | 1.00 | 31.44 | AAAA |
| ATOM | 2822 | CA | ASP | 353 | 21.136 | 51.286 | 66.012 | 1.00 | 26.50 | AAAA |
| ATOM | 2823 | CB | ASP | 353 | 20.543 | 50.635 | 64.746 | 1.00 | 50.09 | AAAA |
| ATOM | 2824 | CG | ASP | 353 | 20.880 | 49.176 | 64.604 | 1.00 | 52.79 | AAAA |
| ATOM | 2825 | OD1 | ASP | 353 | 21.980 | 48.861 | 64.109 | 1.00 | 58.55 | AAAA |
| ATOM | 2826 | OD2 | ASP | 353 | 20.040 | 48.339 | 64.984 | 1.00 | 73.19 | AAAA |
| ATOM | 2827 | C | ASP | 353 | 20.328 | 50.930 | 67.257 | 1.00 | 26.41 | AAAA |
| ATOM | 2828 | O | ASP | 353 | 20.806 | 50.214 | 68.136 | 1.00 | 25.73 | AAAA |
| ATOM | 2829 | N | PRO | 354 | 19.118 | 51.481 | 67.385 | 1.00 | 30.12 | AAAA |
| ATOM | 2830 | CD | PRO | 354 | 18.428 | 52.429 | 66.495 | 1.00 | 35.38 | AAAA |
| ATOM | 2831 | CA | PRO | 354 | 18.276 | 51.190 | 68.547 | 1.00 | 34.02 | AAAA |
| ATOM | 2832 | CB | PRO | 354 | 17.091 | 52.129 | 68.340 | 1.00 | 32.25 | AAAA |
| ATOM | 2833 | CG | PRO | 354 | 16.974 | 52.139 | 66.833 | 1.00 | 44.48 | AAAA |
| ATOM | 2834 | C | PRO | 354 | 17.838 | 49.736 | 68.512 | 1.00 | 34.00 | AAAA |
| ATOM | 2835 | O | PRO | 354 | 17.829 | 49.111 | 67.452 | 1.00 | 28.28 | AAAA |
| ATOM | 2836 | N | TRP | 355 | 17.484 | 49.190 | 69.664 | 1.00 | 23.89 | AAAA |
| ATOM | 2837 | CA | TRP | 355 | 17.010 | 47.818 | 69.669 | 1.00 | 33.84 | AAAA |
| ATOM | 2838 | CB | TRP | 355 | 16.653 | 47.363 | 71.076 | 1.00 | 33.84 | AAAA |

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Figure 16-44

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2839 | CG | TRP | 355 | 17.844 | 46.946 | 71.832 | 1.00 | 49.97 | AAAA |
| ATOM | 2840 | CD2 | TRP | 355 | 18.364 | 45.622 | 71.905 | 1.00 | 46.60 | AAAA |
| ATOM | 2841 | CE2 | TRP | 355 | 19.567 | 45.682 | 72.639 | 1.00 | 54.73 | AAAA |
| ATOM | 2842 | CE3 | TRP | 355 | 17.931 | 44.386 | 71.419 | 1.00 | 46.90 | AAAA |
| ATOM | 2843 | CD1 | TRP | 355 | 18.723 | 47.746 | 72.507 | 1.00 | 56.10 | AAAA |
| ATOM | 2844 | NE1 | TRP | 355 | 19.765 | 46.991 | 72.997 | 1.00 | 56.07 | AAAA |
| ATOM | 2845 | CZ2 | TRP | 355 | 20.340 | 44.552 | 72.897 | 1.00 | 55.25 | AAAA |
| ATOM | 2846 | CZ3 | TRP | 355 | 18.696 | 43.267 | 71.674 | 1.00 | 50.74 | AAAA |
| ATOM | 2847 | CH2 | TRP | 355 | 19.887 | 43.356 | 72.405 | 1.00 | 50.68 | AAAA |
| ATOM | 2848 | C | TRP | 355 | 15.789 | 47.712 | 68.776 | 1.00 | 33.12 | AAAA |
| ATOM | 2849 | O | TRP | 355 | 15.096 | 48.705 | 68.550 | 1.00 | 29.41 | AAAA |
| ATOM | 2850 | N | ARG | 356 | 15.547 | 46.508 | 68.263 | 1.00 | 23.90 | AAAA |
| ATOM | 2851 | CA | ARG | 356 | 14.413 | 46.237 | 67.387 | 1.00 | 23.96 | AAAA |
| ATOM | 2852 | CB | ARG | 356 | 14.892 | 46.096 | 65.935 | 1.00 | 22.66 | AAAA |
| ATOM | 2853 | CG | ARG | 356 | 15.505 | 47.385 | 65.393 | 1.00 | 29.06 | AAAA |
| ATOM | 2854 | CD | ARG | 356 | 16.291 | 47.212 | 64.108 | 1.00 | 28.92 | AAAA |
| ATOM | 2855 | NE | ARG | 356 | 16.833 | 48.503 | 63.686 | 1.00 | 24.73 | AAAA |
| ATOM | 2856 | CZ | ARG | 356 | 17.733 | 48.668 | 62.724 | 1.00 | 23.57 | AAAA |
| ATOM | 2857 | NH1 | ARG | 356 | 18.209 | 47.616 | 62.066 | 1.00 | 22.15 | AAAA |
| ATOM | 2858 | NH2 | ARG | 356 | 18.153 | 49.891 | 62.418 | 1.00 | 22.69 | AAAA |
| ATOM | 2859 | C | ARG | 356 | 13.781 | 44.944 | 67.878 | 1.00 | 24.89 | AAAA |
| ATOM | 2860 | O | ARG | 356 | 13.785 | 43.925 | 67.189 | 1.00 | 22.25 | AAAA |
| ATOM | 2861 | N | GLY | 357 | 13.231 | 44.993 | 69.085 | 1.00 | 23.91 | AAAA |
| ATOM | 2862 | CA | GLY | 357 | 12.631 | 43.805 | 69.657 | 1.00 | 26.72 | AAAA |
| ATOM | 2863 | C | GLY | 357 | 11.138 | 43.671 | 69.465 | 1.00 | 26.90 | AAAA |
| ATOM | 2864 | O | GLY | 357 | 10.536 | 44.330 | 68.619 | 1.00 | 29.87 | AAAA |
| ATOM | 2865 | N | GLY | 358 | 10.544 | 42.797 | 70.265 | 1.00 | 28.22 | AAAA |
| ATOM | 2866 | CA | GLY | 358 | 9.118 | 42.561 | 70.188 | 1.00 | 30.96 | AAAA |
| ATOM | 2867 | C | GLY | 358 | 8.800 | 41.274 | 70.920 | 1.00 | 30.03 | AAAA |
| ATOM | 2868 | O | GLY | 358 | 9.626 | 40.757 | 71.663 | 1.00 | 24.03 | AAAA |
| ATOM | 2869 | N | GLU | 359 | 7.601 | 40.747 | 70.715 | 1.00 | 28.34 | AAAA |
| ATOM | 2870 | CA | GLU | 359 | 7.218 | 39.509 | 71.366 | 1.00 | 24.37 | AAAA |
| ATOM | 2871 | CB | GLU | 359 | 5.699 | 39.372 | 71.375 | 1.00 | 32.52 | AAAA |
| ATOM | 2872 | CG | GLU | 359 | 4.981 | 40.327 | 72.299 | 1.00 | 45.44 | AAAA |
| ATOM | 2873 | CD | GLU | 359 | 3.472 | 40.250 | 72.132 | 1.00 | 50.43 | AAAA |
| ATOM | 2874 | OE1 | GLU | 359 | 2.924 | 39.125 | 72.151 | 1.00 | 42.92 | AAAA |
| ATOM | 2875 | OE2 | GLU | 359 | 2.839 | 41.316 | 71.987 | 1.00 | 40.72 | AAAA |
| ATOM | 2876 | C | GLU | 359 | 7.804 | 38.323 | 70.628 | 1.00 | 27.35 | AAAA |
| ATOM | 2877 | O | GLU | 359 | 8.138 | 38.415 | 69.449 | 1.00 | 22.94 | AAAA |
| ATOM | 2878 | N | VAL | 360 | 7.944 | 37.208 | 71.325 | 1.00 | 19.68 | AAAA |
| ATOM | 2879 | CA | VAL | 360 | 8.441 | 36.017 | 70.672 | 1.00 | 21.28 | AAAA |
| ATOM | 2880 | CB | VAL | 360 | 9.300 | 35.188 | 71.621 | 1.00 | 26.71 | AAAA |
| ATOM | 2881 | CG1 | VAL | 360 | 9.783 | 33.917 | 70.912 | 1.00 | 20.64 | AAAA |
| ATOM | 2882 | CG2 | VAL | 360 | 10.486 | 36.038 | 72.113 | 1.00 | 25.79 | AAAA |
| ATOM | 2883 | C | VAL | 360 | 7.228 | 35.202 | 70.197 | 1.00 | 25.51 | AAAA |
| ATOM | 2884 | O | VAL | 360 | 6.442 | 34.700 | 71.011 | 1.00 | 19.75 | AAAA |
| ATOM | 2885 | N | ARG | 361 | 7.065 | 35.094 | 68.875 | 1.00 | 18.48 | AAAA |
| ATOM | 2886 | CA | ARG | 361 | 5.947 | 34.337 | 68.307 | 1.00 | 22.01 | AAAA |
| ATOM | 2887 | CB | ARG | 361 | 5.988 | 34.389 | 66.772 | 1.00 | 19.31 | AAAA |
| ATOM | 2888 | CG | ARG | 361 | 5.446 | 35.671 | 66.204 | 1.00 | 30.86 | AAAA |
| ATOM | 2889 | CD | ARG | 361 | 5.735 | 35.730 | 64.723 | 1.00 | 37.95 | AAAA |
| ATOM | 2890 | NE | ARG | 361 | 7.111 | 36.148 | 64.460 | 1.00 | 30.73 | AAAA |
| ATOM | 2891 | CZ | ARG | 361 | 7.616 | 36.275 | 63.242 | 1.00 | 22.89 | AAAA |
| ATOM | 2892 | NH1 | ARG | 361 | 6.851 | 36.006 | 62.186 | 1.00 | 19.02 | AAAA |
| ATOM | 2893 | NH2 | ARG | 361 | 8.861 | 36.704 | 63.081 | 1.00 | 23.47 | AAAA |
| ATOM | 2894 | C | ARG | 361 | 5.897 | 32.879 | 68.714 | 1.00 | 26.11 | AAAA |
| ATOM | 2895 | O | ARG | 361 | 6.926 | 32.255 | 68.968 | 1.00 | 21.79 | AAAA |
| ATOM | 2896 | N | LYS | 362 | 4.681 | 32.338 | 68.763 | 1.00 | 24.89 | AAAA |
| ATOM | 2897 | CA | LYS | 362 | 4.479 | 30.938 | 69.125 | 1.00 | 28.63 | AAAA |
| ATOM | 2898 | CB | LYS | 362 | 2.961 | 30.570 | 69.070 | 1.00 | 22.91 | AAAA |
| ATOM | 2899 | CG | LYS | 362 | 2.145 | 31.200 | 70.168 | 1.00 | 50.86 | AAAA |
| ATOM | 2900 | CD | LYS | 362 | 2.290 | 32.715 | 70.157 | 1.00 | 57.51 | AAAA |
| ATOM | 2901 | CE | LYS | 362 | 1.923 | 33.278 | 68.799 | 1.00 | 50.87 | AAAA |
| ATOM | 2902 | NZ | LYS | 362 | 2.307 | 34.683 | 68.711 | 1.00 | 22.99 | AAAA |
| ATOM | 2903 | C | LYS | 362 | 5.269 | 30.014 | 68.202 | 1.00 | 16.77 | AAAA |
| ATOM | 2904 | O | LYS | 362 | 5.808 | 29.007 | 68.647 | 1.00 | 22.90 | AAAA |

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Figure 16-45

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2905 | N | GLU | 363 | 5.311 | 30.355 | 66.913 | 1.00 | 25.24 | AAAA |
| ATOM | 2906 | CA | GLU | 363 | 6.055 | 29.577 | 65.910 | 1.00 | 26.29 | AAAA |
| ATOM | 2907 | CB | GLU | 363 | 6.207 | 30.342 | 64.608 | 1.00 | 33.50 | AAAA |
| ATOM | 2908 | CG | GLU | 363 | 4.999 | 30.639 | 63.824 | 1.00 | 48.73 | AAAA |
| ATOM | 2909 | CD | GLU | 363 | 5.368 | 31.494 | 62.638 | 1.00 | 42.01 | AAAA |
| ATOM | 2910 | OE1 | GLU | 363 | 6.299 | 31.087 | 61.895 | 1.00 | 28.50 | AAAA |
| ATOM | 2911 | OE2 | GLU | 363 | 4.738 | 32.558 | 62.461 | 1.00 | 44.91 | AAAA |
| ATOM | 2912 | C | GLU | 363 | 7.481 | 29.326 | 66.349 | 1.00 | 19.00 | AAAA |
| ATOM | 2913 | O | GLU | 363 | 8.011 | 28.218 | 66.226 | 1.00 | 18.66 | AAAA |
| ATOM | 2914 | N | VAL | 364 | 8.121 | 30.399 | 66.790 | 1.00 | 20.69 | AAAA |
| ATOM | 2915 | CA | VAL | 364 | 9.501 | 30.303 | 67.219 | 1.00 | 23.13 | AAAA |
| ATOM | 2916 | CB | VAL | 364 | 10.096 | 31.681 | 67.510 | 1.00 | 16.98 | AAAA |
| ATOM | 2917 | CG1 | VAL | 364 | 11.515 | 31.513 | 68.010 | 1.00 | 22.32 | AAAA |
| ATOM | 2918 | CG2 | VAL | 364 | 10.082 | 32.548 | 66.242 | 1.00 | 23.99 | AAAA |
| ATOM | 2919 | C | VAL | 364 | 9.625 | 29.415 | 68.448 | 1.00 | 19.28 | AAAA |
| ATOM | 2920 | O | VAL | 364 | 10.507 | 28.548 | 68.510 | 1.00 | 20.17 | AAAA |
| ATOM | 2921 | N | LYS | 365 | 8.735 | 29.600 | 69.417 | 1.00 | 21.11 | AAAA |
| ATOM | 2922 | CA | LYS | 365 | 8.780 | 28.768 | 70.612 | 1.00 | 18.15 | AAAA |
| ATOM | 2923 | CB | LYS | 365 | 7.711 | 29.210 | 71.626 | 1.00 | 25.22 | AAAA |
| ATOM | 2924 | CG | LYS | 365 | 7.921 | 30.611 | 72.167 | 1.00 | 32.99 | AAAA |
| ATOM | 2925 | CD | LYS | 365 | 6.901 | 30.949 | 73.253 | 1.00 | 36.09 | AAAA |
| ATOM | 2926 | CE | LYS | 365 | 7.121 | 32.357 | 73.790 | 1.00 | 28.99 | AAAA |
| ATOM | 2927 | NZ | LYS | 365 | 6.178 | 32.736 | 74.882 | 1.00 | 38.98 | AAAA |
| ATOM | 2928 | C | LYS | 365 | 8.574 | 27.305 | 70.236 | 1.00 | 19.49 | AAAA |
| ATOM | 2929 | O | LYS | 365 | 9.255 | 26.417 | 70.758 | 1.00 | 22.04 | AAAA |
| ATOM | 2930 | N | ASP | 366 | 7.635 | 27.048 | 69.327 | 1.00 | 22.45 | AAAA |
| ATOM | 2931 | CA | ASP | 366 | 7.386 | 25.669 | 68.915 | 1.00 | 22.62 | AAAA |
| ATOM | 2932 | CB | ASP | 366 | 6.173 | 25.574 | 67.967 | 1.00 | 21.69 | AAAA |
| ATOM | 2933 | CG | ASP | 366 | 4.870 | 25.987 | 68.634 | 1.00 | 27.75 | AAAA |
| ATOM | 2934 | OD1 | ASP | 366 | 4.763 | 25.890 | 69.881 | 1.00 | 31.01 | AAAA |
| ATOM | 2935 | OD2 | ASP | 366 | 3.938 | 26.382 | 67.907 | 1.00 | 33.20 | AAAA |
| ATOM | 2936 | C | ASP | 366 | 8.606 | 25.034 | 68.237 | 1.00 | 24.53 | AAAA |
| ATOM | 2937 | O | ASP | 366 | 8.924 | 23.871 | 68.480 | 1.00 | 21.13 | AAAA |
| ATOM | 2938 | N | THR | 367 | 9.281 | 25.787 | 67.380 | 1.00 | 26.19 | AAAA |
| ATOM | 2939 | CA | THR | 367 | 10.462 | 25.252 | 66.694 | 1.00 | 21.68 | AAAA |
| ATOM | 2940 | CB | THR | 367 | 11.035 | 26.301 | 65.742 | 1.00 | 14.56 | AAAA |
| ATOM | 2941 | OG1 | THR | 367 | 10.085 | 26.545 | 64.697 | 1.00 | 21.76 | AAAA |
| ATOM | 2942 | CG2 | THR | 367 | 12.340 | 25.825 | 65.138 | 1.00 | 19.83 | AAAA |
| ATOM | 2943 | C | THR | 367 | 11.523 | 24.822 | 67.710 | 1.00 | 19.02 | AAAA |
| ATOM | 2944 | O | THR | 367 | 12.071 | 23.717 | 67.625 | 1.00 | 21.79 | AAAA |
| ATOM | 2945 | N | LEU | 368 | 11.802 | 25.684 | 68.683 | 1.00 | 18.42 | AAAA |
| ATOM | 2946 | CA | LEU | 368 | 12.797 | 25.348 | 69.700 | 1.00 | 21.02 | AAAA |
| ATOM | 2947 | CB | LEU | 368 | 13.148 | 26.569 | 70.560 | 1.00 | 17.34 | AAAA |
| ATOM | 2948 | CG | LEU | 368 | 14.206 | 27.518 | 69.959 | 1.00 | 17.45 | AAAA |
| ATOM | 2949 | CD1 | LEU | 368 | 15.525 | 26.758 | 69.817 | 1.00 | 16.83 | AAAA |
| ATOM | 2950 | CD2 | LEU | 368 | 13.756 | 28.041 | 68.593 | 1.00 | 19.49 | AAAA |
| ATOM | 2951 | C | LEU | 368 | 12.361 | 24.189 | 70.589 | 1.00 | 23.17 | AAAA |
| ATOM | 2952 | O | LEU | 368 | 13.203 | 23.420 | 71.052 | 1.00 | 24.81 | AAAA |
| ATOM | 2953 | N | GLU | 369 | 11.059 | 24.055 | 70.839 | 1.00 | 23.97 | AAAA |
| ATOM | 2954 | CA | GLU | 369 | 10.597 | 22.929 | 71.653 | 1.00 | 19.36 | AAAA |
| ATOM | 2955 | CB | GLU | 369 | 9.127 | 23.113 | 72.063 | 1.00 | 21.81 | AAAA |
| ATOM | 2956 | CG | GLU | 369 | 8.913 | 24.225 | 73.100 | 1.00 | 40.15 | AAAA |
| ATOM | 2957 | CD | GLU | 369 | 7.450 | 24.416 | 73.487 | 1.00 | 49.38 | AAAA |
| ATOM | 2958 | OE1 | GLU | 369 | 6.806 | 23.429 | 73.905 | 1.00 | 43.26 | AAAA |
| ATOM | 2959 | OE2 | GLU | 369 | 6.948 | 25.558 | 73.382 | 1.00 | 57.31 | AAAA |
| ATOM | 2960 | C | GLU | 369 | 10.778 | 21.623 | 70.859 | 1.00 | 24.29 | AAAA |
| ATOM | 2961 | O | GLU | 369 | 11.172 | 20.605 | 71.420 | 1.00 | 25.96 | AAAA |
| ATOM | 2962 | N | LYS | 370 | 10.488 | 21.643 | 69.560 | 1.00 | 22.98 | AAAA |
| ATOM | 2963 | CA | LYS | 370 | 10.665 | 20.437 | 68.746 | 1.00 | 23.19 | AAAA |
| ATOM | 2964 | CB | LYS | 370 | 10.051 | 20.596 | 67.347 | 1.00 | 26.83 | AAAA |
| ATOM | 2965 | CG | LYS | 370 | 8.537 | 20.461 | 67.287 | 1.00 | 36.68 | AAAA |
| ATOM | 2966 | CD | LYS | 370 | 8.056 | 20.431 | 65.832 | 1.00 | 39.85 | AAAA |
| ATOM | 2967 | CE | LYS | 370 | 6.567 | 20.105 | 65.740 | 1.00 | 56.23 | AAAA |
| ATOM | 2968 | NZ | LYS | 370 | 6.082 | 19.996 | 64.326 | 1.00 | 56.10 | AAAA |
| ATOM | 2969 | C | LYS | 370 | 12.148 | 20.123 | 68.602 | 1.00 | 31.63 | AAAA |
| ATOM | 2970 | O | LYS | 370 | 12.549 | 18.958 | 68.587 | 1.00 | 36.88 | AAAA |

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Figure 16-46

| | | | | | | | | | | |
|--------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2971 | N | ALA | 371 | 12.961 | 21.170 | 68.491 | 1.00 | 26.25 | AAAA |
| ATOM | 2972 | CA | ALA | 371 | 14.407 | 21.009 | 68.360 | 1.00 | 27.33 | AAAA |
| ATOM | 2973 | CB | ALA | 371 | 15.079 | 22.370 | 68.188 | 1.00 | 23.70 | AAAA |
| ATOM | 2974 | C | ALA | 371 | 14.989 | 20.308 | 69.581 | 1.00 | 26.74 | AAAA |
| ATOM | 2975 | O | ALA | 371 | 15.892 | 19.482 | 69.452 | 1.00 | 29.52 | AAAA |
| ATOM | 2976 | N | ALA | 372 | 14.484 | 20.652 | 70.764 | 1.00 | 24.83 | AAAA |
| ATOM | 2977 | CA | ALA | 372 | 14.959 | 20.055 | 72.012 | 1.00 | 34.24 | AAAA |
| ATOM | 2978 | CB | ALA | 372 | 14.305 | 20.750 | 73.214 | 1.00 | 37.17 | AAAA |
| ATOM | 2979 | C | ALA | 372 | 14.663 | 18.564 | 72.061 | 1.00 | 45.62 | AAAA |
| ATOM | 2980 | O | ALA | 372 | 15.563 | 17.741 | 72.280 | 1.00 | 35.52 | AAAA |
| ATOM | 2981 | N | ALA | 373 | 13.394 | 18.216 | 71.869 | 1.00 | 44.50 | AAAA |
| ATOM | 2982 | CA | ALA | 373 | 13.004 | 16.813 | 71.892 | 1.00 | 49.88 | AAAA |
| ATOM | 2983 | CB | ALA | 373 | 11.506 | 16.681 | 71.628 | 1.00 | 49.32 | AAAA |
| ATOM | 2984 | C | ALA | 373 | 13.807 | 16.072 | 70.825 | 1.00 | 44.64 | AAAA |
| ATOM | 2985 | O | ALA | 373 | 14.669 | 15.250 | 71.201 | 1.00 | 58.19 | AAAA |
| ATOM | 2986 | OXT | ALA | 373 | 13.591 | 16.337 | 69.626 | 1.00 | 41.63 | AAAA |
| HETATM | 2987 | OH2 | WAT | 1 | 36.368 | 43.907 | 49.242 | 1.00 | 13.03 | SOLV |
| HETATM | 2988 | OH2 | WAT | 2 | 23.107 | 30.584 | 59.802 | 1.00 | 11.42 | SOLV |
| HETATM | 2989 | OH2 | WAT | 3 | 20.594 | 33.744 | 61.457 | 1.00 | 14.73 | SOLV |
| HETATM | 2990 | OH2 | WAT | 4 | 31.359 | 16.551 | 51.590 | 1.00 | 19.84 | SOLV |
| HETATM | 2991 | OH2 | WAT | 5 | 30.389 | 18.140 | 45.769 | 1.00 | 19.94 | SOLV |
| HETATM | 2992 | OH2 | WAT | 6 | 16.925 | 41.748 | 56.551 | 1.00 | 13.33 | SOLV |
| HETATM | 2993 | OH2 | WAT | 7 | 28.448 | 16.084 | 62.316 | 1.00 | 14.08 | SOLV |
| HETATM | 2994 | OH2 | WAT | 8 | 40.375 | 38.476 | 55.678 | 1.00 | 19.10 | SOLV |
| HETATM | 2995 | OH2 | WAT | 9 | 18.455 | 29.667 | 54.797 | 1.00 | 18.81 | SOLV |
| HETATM | 2996 | OH2 | WAT | 10 | 26.305 | 18.390 | 59.507 | 1.00 | 16.65 | SOLV |
| HETATM | 2997 | OH2 | WAT | 11 | 50.145 | 32.063 | 58.142 | 1.00 | 16.53 | SOLV |
| HETATM | 2998 | OH2 | WAT | 12 | 45.935 | 30.996 | 40.672 | 1.00 | 25.08 | SOLV |
| HETATM | 2999 | OH2 | WAT | 13 | 26.358 | 43.110 | 74.179 | 1.00 | 22.91 | SOLV |
| HETATM | 3000 | OH2 | WAT | 14 | 48.727 | 24.720 | 56.917 | 1.00 | 25.49 | SOLV |
| HETATM | 3001 | OH2 | WAT | 15 | 30.244 | 18.663 | 50.165 | 1.00 | 25.78 | SOLV |
| HETATM | 3002 | OH2 | WAT | 16 | 10.615 | 28.799 | 63.631 | 1.00 | 22.40 | SOLV |
| HETATM | 3003 | OH2 | WAT | 17 | 18.401 | 20.018 | 62.704 | 1.00 | 21.46 | SOLV |
| HETATM | 3004 | OH2 | WAT | 18 | 22.195 | 47.791 | 60.896 | 1.00 | 26.19 | SOLV |
| HETATM | 3005 | OH2 | WAT | 19 | 3.278 | 32.141 | 65.350 | 1.00 | 20.38 | SOLV |
| HETATM | 3006 | OH2 | WAT | 20 | 23.643 | 22.897 | 59.512 | 1.00 | 21.27 | SOLV |
| HETATM | 3007 | OH2 | WAT | 21 | 50.287 | 23.101 | 48.818 | 1.00 | 19.73 | SOLV |
| HETATM | 3008 | OH2 | WAT | 22 | 44.725 | 34.256 | 46.541 | 1.00 | 18.74 | SOLV |
| HETATM | 3009 | OH2 | WAT | 23 | 8.346 | 30.527 | 49.922 | 1.00 | 22.33 | SOLV |
| HETATM | 3010 | OH2 | WAT | 24 | 39.855 | 33.795 | 67.390 | 1.00 | 20.43 | SOLV |
| HETATM | 3011 | OH2 | WAT | 25 | 7.827 | 32.763 | 57.779 | 1.00 | 19.24 | SOLV |
| HETATM | 3012 | OH2 | WAT | 26 | 45.388 | 34.567 | 36.246 | 1.00 | 20.86 | SOLV |
| HETATM | 3013 | OH2 | WAT | 27 | 47.636 | 32.244 | 33.388 | 1.00 | 20.41 | SOLV |
| HETATM | 3014 | OH2 | WAT | 28 | 32.514 | 35.684 | 41.278 | 1.00 | 24.76 | SOLV |
| HETATM | 3015 | OH2 | WAT | 29 | 26.188 | 15.341 | 61.913 | 1.00 | 19.63 | SOLV |
| HETATM | 3016 | OH2 | WAT | 30 | 14.957 | 43.169 | 56.333 | 1.00 | 23.80 | SOLV |
| HETATM | 3017 | OH2 | WAT | 31 | 24.483 | 43.556 | 55.704 | 1.00 | 27.25 | SOLV |
| HETATM | 3018 | OH2 | WAT | 32 | 41.141 | 16.376 | 48.456 | 1.00 | 25.99 | SOLV |
| HETATM | 3019 | OH2 | WAT | 33 | 23.104 | 17.625 | 54.086 | 1.00 | 26.37 | SOLV |
| HETATM | 3020 | OH2 | WAT | 34 | 51.301 | 28.602 | 57.694 | 1.00 | 32.78 | SOLV |
| HETATM | 3021 | OH2 | WAT | 35 | 51.376 | 29.469 | 53.156 | 1.00 | 24.27 | SOLV |
| HETATM | 3022 | OH2 | WAT | 36 | 12.518 | 22.131 | 49.816 | 1.00 | 23.60 | SOLV |
| HETATM | 3023 | OH2 | WAT | 37 | 6.521 | 27.442 | 50.861 | 1.00 | 25.87 | SOLV |
| HETATM | 3024 | OH2 | WAT | 38 | 30.390 | 33.757 | 34.190 | 1.00 | 19.87 | SOLV |
| HETATM | 3025 | OH2 | WAT | 39 | 8.328 | 29.586 | 62.062 | 1.00 | 32.01 | SOLV |
| HETATM | 3026 | OH2 | WAT | 40 | 30.180 | 24.235 | 30.724 | 1.00 | 22.61 | SOLV |
| HETATM | 3027 | OH2 | WAT | 41 | 44.521 | 30.663 | 38.395 | 1.00 | 27.52 | SOLV |
| HETATM | 3028 | OH2 | WAT | 42 | 30.981 | 18.043 | 41.186 | 1.00 | 23.45 | SOLV |
| HETATM | 3029 | OH2 | WAT | 43 | 14.632 | 37.127 | 73.830 | 1.00 | 29.36 | SOLV |
| HETATM | 3030 | OH2 | WAT | 44 | 39.332 | 25.953 | 72.230 | 1.00 | 21.87 | SOLV |
| HETATM | 3031 | OH2 | WAT | 45 | 7.597 | 37.592 | 51.896 | 1.00 | 39.62 | SOLV |
| HETATM | 3032 | OH2 | WAT | 46 | 15.027 | 18.079 | 54.827 | 1.00 | 26.65 | SOLV |
| HETATM | 3033 | OH2 | WAT | 47 | 11.076 | 45.493 | 66.435 | 1.00 | 38.18 | SOLV |
| HETATM | 3034 | OH2 | WAT | 48 | 42.124 | 18.055 | 37.233 | 1.00 | 28.62 | SOLV |
| HETATM | 3035 | OH2 | WAT | 49 | 48.736 | 25.764 | 64.149 | 1.00 | 31.88 | SOLV |
| HETATM | 3036 | OH2 | WAT | 50 | 50.383 | 27.254 | 54.972 | 1.00 | 24.36 | SOLV |

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Figure 16-47

| | | | | | | | | | | |
|--------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| HETATM | 3037 | OH2 | WAT | 51 | 48.659 | 36.025 | 68.226 | 1.00 | 33.89 | SOLV |
| HETATM | 3038 | OH2 | WAT | 52 | 36.998 | 27.228 | 71.440 | 1.00 | 21.03 | SOLV |
| HETATM | 3039 | OH2 | WAT | 53 | 41.303 | 16.309 | 55.307 | 1.00 | 32.23 | SOLV |
| HETATM | 3040 | OH2 | WAT | 54 | 33.242 | 39.524 | 49.454 | 1.00 | 29.77 | SOLV |
| HETATM | 3041 | OH2 | WAT | 55 | 45.004 | 25.973 | 35.031 | 1.00 | 21.59 | SOLV |
| HETATM | 3042 | OH2 | WAT | 56 | 19.039 | 25.829 | 45.793 | 1.00 | 33.48 | SOLV |
| HETATM | 3043 | OH2 | WAT | 57 | 17.922 | 35.542 | 50.154 | 1.00 | 37.51 | SOLV |
| HETATM | 3044 | OH2 | WAT | 58 | 10.409 | 26.864 | 73.166 | 1.00 | 26.54 | SOLV |
| HETATM | 3045 | OH2 | WAT | 59 | 11.835 | 22.805 | 59.408 | 1.00 | 20.83 | SOLV |
| HETATM | 3046 | OH2 | WAT | 60 | 18.254 | 48.699 | 53.224 | 1.00 | 28.41 | SOLV |
| HETATM | 3047 | OH2 | WAT | 61 | 10.426 | 26.647 | 60.447 | 1.00 | 32.72 | SOLV |
| HETATM | 3048 | OH2 | WAT | 62 | 21.304 | 55.086 | 63.510 | 1.00 | 28.84 | SOLV |
| HETATM | 3049 | OH2 | WAT | 63 | 32.532 | 51.211 | 45.469 | 1.00 | 32.48 | SOLV |
| HETATM | 3050 | OH2 | WAT | 64 | 22.658 | 61.079 | 57.420 | 1.00 | 27.32 | SOLV |
| HETATM | 3051 | OH2 | WAT | 65 | 16.734 | 24.334 | 74.721 | 1.00 | 27.44 | SOLV |
| HETATM | 3052 | OH2 | WAT | 66 | 32.758 | 37.824 | 54.391 | 1.00 | 25.07 | SOLV |
| HETATM | 3053 | OH2 | WAT | 67 | 11.142 | 25.859 | 49.706 | 1.00 | 29.66 | SOLV |
| HETATM | 3054 | OH2 | WAT | 68 | 24.192 | 15.261 | 53.236 | 1.00 | 30.21 | SOLV |
| HETATM | 3055 | OH2 | WAT | 69 | 19.816 | 17.916 | 66.357 | 1.00 | 30.50 | SOLV |
| HETATM | 3056 | OH2 | WAT | 70 | 50.347 | 23.975 | 53.197 | 1.00 | 28.08 | SOLV |
| HETATM | 3057 | OH2 | WAT | 71 | 50.258 | 30.918 | 51.113 | 1.00 | 20.19 | SOLV |
| HETATM | 3058 | OH2 | WAT | 72 | 21.047 | 17.624 | 68.693 | 1.00 | 41.23 | SOLV |
| HETATM | 3059 | OH2 | WAT | 73 | 26.782 | 33.756 | 49.995 | 1.00 | 25.80 | SOLV |
| HETATM | 3060 | OH2 | WAT | 74 | 12.570 | 43.844 | 64.441 | 1.00 | 31.03 | SOLV |
| HETATM | 3061 | OH2 | WAT | 75 | 35.555 | 41.287 | 50.852 | 1.00 | 24.03 | SOLV |
| HETATM | 3062 | OH2 | WAT | 76 | 27.764 | 18.231 | 61.827 | 1.00 | 18.28 | SOLV |
| HETATM | 3063 | OH2 | WAT | 77 | 26.715 | 29.236 | 38.391 | 1.00 | 23.18 | SOLV |
| HETATM | 3064 | OH2 | WAT | 78 | 21.461 | 23.245 | 48.872 | 1.00 | 23.80 | SOLV |
| HETATM | 3065 | OH2 | WAT | 79 | 49.246 | 28.263 | 65.477 | 1.00 | 21.52 | SOLV |
| HETATM | 3066 | OH2 | WAT | 80 | 31.785 | 13.301 | 69.606 | 1.00 | 31.11 | SOLV |
| HETATM | 3067 | OH2 | WAT | 81 | 49.811 | 34.740 | 59.229 | 1.00 | 31.76 | SOLV |
| HETATM | 3068 | OH2 | WAT | 82 | 45.670 | 33.188 | 42.470 | 1.00 | 23.13 | SOLV |
| HETATM | 3069 | OH2 | WAT | 83 | 9.408 | 39.751 | 55.872 | 1.00 | 31.53 | SOLV |
| HETATM | 3070 | OH2 | WAT | 84 | 35.166 | 35.878 | 29.899 | 1.00 | 37.32 | SOLV |
| HETATM | 3071 | OH2 | WAT | 85 | 41.927 | 22.970 | 73.694 | 1.00 | 44.07 | SOLV |
| HETATM | 3072 | OH2 | WAT | 86 | 22.125 | 34.577 | 49.199 | 1.00 | 44.65 | SOLV |
| HETATM | 3073 | OH2 | WAT | 87 | 43.984 | 33.541 | 37.965 | 1.00 | 24.88 | SOLV |
| HETATM | 3074 | OH2 | WAT | 88 | 11.997 | 17.962 | 56.312 | 1.00 | 34.85 | SOLV |
| HETATM | 3075 | OH2 | WAT | 89 | 42.194 | 14.737 | 59.766 | 1.00 | 25.91 | SOLV |
| HETATM | 3076 | OH2 | WAT | 90 | 49.313 | 24.200 | 41.684 | 1.00 | 29.29 | SOLV |
| HETATM | 3077 | OH2 | WAT | 91 | 48.504 | 33.595 | 61.519 | 1.00 | 30.32 | SOLV |
| HETATM | 3078 | OH2 | WAT | 92 | 24.773 | 18.356 | 33.365 | 1.00 | 53.13 | SOLV |
| HETATM | 3079 | OH2 | WAT | 93 | 35.160 | 35.656 | 47.470 | 1.00 | 41.41 | SOLV |
| HETATM | 3080 | OH2 | WAT | 94 | 44.682 | 36.658 | 39.962 | 1.00 | 29.24 | SOLV |
| HETATM | 3081 | OH2 | WAT | 95 | 9.576 | 41.033 | 52.549 | 1.00 | 51.83 | SOLV |
| HETATM | 3082 | OH2 | WAT | 96 | 47.199 | 20.112 | 42.102 | 1.00 | 40.39 | SOLV |
| HETATM | 3083 | OH2 | WAT | 97 | 49.254 | 26.331 | 59.641 | 1.00 | 37.03 | SOLV |
| HETATM | 3084 | OH2 | WAT | 98 | 26.808 | 37.600 | 38.172 | 1.00 | 28.74 | SOLV |
| HETATM | 3085 | OH2 | WAT | 99 | 40.749 | 14.572 | 64.635 | 1.00 | 33.42 | SOLV |
| HETATM | 3086 | OH2 | WAT | 100 | 24.850 | 44.161 | 47.775 | 1.00 | 27.89 | SOLV |
| HETATM | 3087 | OH2 | WAT | 101 | 34.326 | 42.063 | 46.714 | 1.00 | 42.22 | SOLV |
| HETATM | 3088 | OH2 | WAT | 102 | 30.226 | 34.544 | 52.026 | 1.00 | 30.77 | SOLV |
| HETATM | 3089 | OH2 | WAT | 103 | 47.824 | 39.054 | 78.097 | 1.00 | 52.16 | SOLV |
| HETATM | 3090 | OH2 | WAT | 104 | 19.665 | 18.953 | 47.438 | 1.00 | 51.70 | SOLV |
| HETATM | 3091 | OH2 | WAT | 105 | 46.857 | 36.525 | 46.232 | 1.00 | 23.65 | SOLV |
| HETATM | 3092 | OH2 | WAT | 106 | 48.069 | 19.460 | 67.360 | 1.00 | 37.56 | SOLV |
| HETATM | 3093 | OH2 | WAT | 107 | 15.553 | 56.850 | 61.838 | 1.00 | 46.95 | SOLV |
| HETATM | 3094 | OH2 | WAT | 108 | 44.026 | 19.119 | 70.671 | 1.00 | 39.55 | SOLV |
| HETATM | 3095 | OH2 | WAT | 109 | 8.139 | 42.064 | 65.674 | 1.00 | 42.61 | SOLV |
| HETATM | 3096 | OH2 | WAT | 110 | 50.624 | 36.591 | 65.779 | 1.00 | 31.59 | SOLV |
| HETATM | 3097 | OH2 | WAT | 111 | 51.398 | 26.073 | 61.043 | 1.00 | 49.09 | SOLV |
| HETATM | 3098 | OH2 | WAT | 112 | 26.174 | 33.692 | 33.551 | 1.00 | 36.61 | SOLV |
| HETATM | 3099 | OH2 | WAT | 113 | 23.545 | 20.203 | 53.001 | 1.00 | 24.34 | SOLV |
| HETATM | 3100 | OH2 | WAT | 114 | 9.083 | 42.965 | 57.697 | 1.00 | 33.65 | SOLV |
| HETATM | 3101 | OH2 | WAT | 115 | 8.442 | 39.898 | 64.594 | 1.00 | 31.21 | SOLV |
| HETATM | 3102 | OH2 | WAT | 116 | 15.219 | 35.897 | 51.951 | 1.00 | 26.59 | SOLV |

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Figure 16-48

| | | | | | | | | |
|-------------|---------|-----|--------|--------|--------|------|-------|------|
| HETATM 3103 | OH2 WAT | 117 | 15.417 | 38.438 | 50.473 | 1.00 | 34.46 | SOLV |
| HETATM 3104 | OH2 WAT | 118 | 40.757 | 26.310 | 29.206 | 1.00 | 29.12 | SOLV |
| HETATM 3105 | OH2 WAT | 119 | 27.717 | 18.542 | 46.553 | 1.00 | 28.17 | SOLV |
| HETATM 3106 | OH2 WAT | 120 | 18.612 | 13.786 | 56.845 | 1.00 | 38.56 | SOLV |
| HETATM 3107 | OH2 WAT | 121 | 43.198 | 31.377 | 72.139 | 1.00 | 26.31 | SOLV |
| HETATM 3108 | OH2 WAT | 122 | 44.188 | 35.704 | 33.802 | 1.00 | 29.81 | SOLV |
| HETATM 3109 | OH2 WAT | 123 | 50.736 | 40.909 | 58.456 | 1.00 | 32.40 | SOLV |
| HETATM 3110 | OH2 WAT | 124 | 31.302 | 33.760 | 31.742 | 1.00 | 30.84 | SOLV |
| HETATM 3111 | OH2 WAT | 125 | 36.895 | 21.264 | 34.198 | 1.00 | 34.67 | SOLV |
| HETATM 3112 | OH2 WAT | 126 | 47.474 | 22.252 | 67.427 | 1.00 | 34.35 | SOLV |
| HETATM 3113 | OH2 WAT | 127 | 7.178 | 25.936 | 64.063 | 1.00 | 31.77 | SOLV |
| HETATM 3114 | OH2 WAT | 128 | 36.362 | 66.647 | 54.021 | 1.00 | 36.88 | SOLV |
| HETATM 3115 | OH2 WAT | 129 | 42.486 | 35.503 | 30.348 | 1.00 | 26.61 | SOLV |
| HETATM 3116 | OH2 WAT | 130 | 8.432 | 34.383 | 50.442 | 1.00 | 37.45 | SOLV |
| HETATM 3117 | OH2 WAT | 131 | 37.644 | 49.018 | 48.946 | 1.00 | 37.33 | SOLV |
| HETATM 3118 | OH2 WAT | 132 | 50.273 | 41.645 | 63.380 | 1.00 | 37.33 | SOLV |
| HETATM 3119 | OH2 WAT | 133 | 7.518 | 26.633 | 61.571 | 1.00 | 45.42 | SOLV |
| HETATM 3120 | OH2 WAT | 134 | 31.483 | 46.197 | 72.538 | 1.00 | 28.02 | SOLV |
| HETATM 3121 | OH2 WAT | 135 | 41.501 | 16.604 | 58.054 | 1.00 | 32.78 | SOLV |
| HETATM 3122 | OH2 WAT | 136 | 45.898 | 47.740 | 55.185 | 1.00 | 43.47 | SOLV |
| HETATM 3123 | OH2 WAT | 137 | 16.300 | 33.614 | 49.519 | 1.00 | 30.37 | SOLV |
| HETATM 3124 | OH2 WAT | 138 | 51.148 | 36.946 | 55.148 | 1.00 | 46.34 | SOLV |
| HETATM 3125 | OH2 WAT | 139 | 21.525 | 53.761 | 50.892 | 1.00 | 38.27 | SOLV |
| HETATM 3126 | OH2 WAT | 140 | 21.603 | 54.580 | 68.690 | 1.00 | 33.10 | SOLV |
| HETATM 3127 | OH2 WAT | 141 | 10.191 | 29.237 | 60.325 | 1.00 | 30.24 | SOLV |
| HETATM 3128 | OH2 WAT | 142 | 16.951 | 18.120 | 66.901 | 1.00 | 40.85 | SOLV |
| HETATM 3129 | OH2 WAT | 143 | 4.943 | 24.912 | 51.199 | 1.00 | 49.13 | SOLV |
| HETATM 3130 | OH2 WAT | 144 | 10.711 | 25.291 | 58.177 | 1.00 | 30.72 | SOLV |
| HETATM 3131 | OH2 WAT | 145 | 30.815 | 43.398 | 36.040 | 1.00 | 42.23 | SOLV |
| HETATM 3132 | OH2 WAT | 146 | 21.763 | 24.512 | 46.695 | 1.00 | 28.31 | SOLV |
| HETATM 3133 | OH2 WAT | 147 | 51.788 | 33.122 | 50.887 | 1.00 | 26.15 | SOLV |
| HETATM 3134 | OH2 WAT | 148 | 24.531 | 44.741 | 72.420 | 1.00 | 27.99 | SOLV |
| HETATM 3135 | OH2 WAT | 149 | 50.938 | 23.483 | 60.422 | 1.00 | 38.20 | SOLV |
| HETATM 3136 | OH2 WAT | 150 | 24.860 | 47.932 | 61.067 | 1.00 | 18.89 | SOLV |
| HETATM 3137 | OH2 WAT | 151 | 27.336 | 37.304 | 35.642 | 1.00 | 33.58 | SOLV |
| HETATM 3138 | OH2 WAT | 152 | 38.680 | 35.535 | 35.974 | 1.00 | 26.89 | SOLV |
| HETATM 3139 | OH2 WAT | 153 | 24.441 | 16.097 | 33.317 | 1.00 | 48.33 | SOLV |
| HETATM 3140 | OH2 WAT | 154 | 20.343 | 18.124 | 73.416 | 1.00 | 36.28 | SOLV |
| HETATM 3141 | OH2 WAT | 155 | 49.765 | 37.948 | 74.801 | 1.00 | 48.41 | SOLV |
| HETATM 3142 | OH2 WAT | 156 | 34.329 | 31.169 | 47.547 | 1.00 | 25.33 | SOLV |
| HETATM 3143 | OH2 WAT | 157 | 43.028 | 24.554 | 72.536 | 1.00 | 41.54 | SOLV |
| HETATM 3144 | OH2 WAT | 158 | 39.888 | 15.082 | 42.035 | 1.00 | 28.76 | SOLV |
| HETATM 3145 | OH2 WAT | 159 | 41.886 | 20.780 | 73.179 | 1.00 | 51.03 | SOLV |
| HETATM 3146 | OH2 WAT | 160 | 22.962 | 49.969 | 58.518 | 1.00 | 35.04 | SOLV |
| HETATM 3147 | OH2 WAT | 161 | 14.696 | 15.261 | 68.016 | 1.00 | 55.47 | SOLV |
| HETATM 3148 | OH2 WAT | 162 | 14.915 | 18.181 | 64.866 | 1.00 | 42.00 | SOLV |
| HETATM 3149 | OH2 WAT | 163 | 30.608 | 49.029 | 52.612 | 1.00 | 47.32 | SOLV |
| HETATM 3150 | OH2 WAT | 164 | 52.566 | 30.906 | 57.612 | 1.00 | 36.71 | SOLV |
| HETATM 3151 | OH2 WAT | 165 | 23.699 | 27.331 | 77.729 | 1.00 | 32.22 | SOLV |
| HETATM 3152 | OH2 WAT | 166 | 36.971 | 59.046 | 63.272 | 1.00 | 43.05 | SOLV |
| HETATM 3153 | OH2 WAT | 167 | 46.053 | 45.927 | 52.876 | 1.00 | 33.66 | SOLV |
| HETATM 3154 | OH2 WAT | 168 | 42.780 | 49.151 | 58.106 | 1.00 | 44.63 | SOLV |
| HETATM 3155 | OH2 WAT | 169 | 15.100 | 44.506 | 72.183 | 1.00 | 45.43 | SOLV |
| HETATM 3156 | OH2 WAT | 170 | 31.677 | 60.998 | 50.050 | 1.00 | 34.51 | SOLV |
| HETATM 3157 | OH2 WAT | 171 | 25.336 | 45.674 | 45.578 | 1.00 | 55.85 | SOLV |
| HETATM 3158 | OH2 WAT | 172 | 17.481 | 18.266 | 49.018 | 1.00 | 32.73 | SOLV |
| HETATM 3159 | OH2 WAT | 173 | 26.112 | 18.147 | 31.404 | 1.00 | 49.94 | SOLV |
| HETATM 3160 | OH2 WAT | 174 | 45.874 | 43.142 | 70.985 | 1.00 | 32.89 | SOLV |
| HETATM 3161 | OH2 WAT | 175 | 34.517 | 17.884 | 33.278 | 1.00 | 42.20 | SOLV |
| HETATM 3162 | OH2 WAT | 176 | 16.330 | 54.886 | 50.466 | 1.00 | 40.74 | SOLV |
| HETATM 3163 | OH2 WAT | 177 | 31.400 | 51.087 | 74.689 | 1.00 | 38.56 | SOLV |
| HETATM 3164 | OH2 WAT | 178 | 50.971 | 27.079 | 67.130 | 1.00 | 44.49 | SOLV |
| HETATM 3165 | OH2 WAT | 179 | 7.933 | 23.412 | 54.691 | 1.00 | 42.84 | SOLV |
| HETATM 3166 | OH2 WAT | 180 | 33.498 | 47.596 | 73.612 | 1.00 | 35.99 | SOLV |
| HETATM 3167 | OH2 WAT | 181 | 26.016 | 19.583 | 44.954 | 1.00 | 51.31 | SOLV |
| HETATM 3168 | OH2 WAT | 182 | 40.139 | 17.026 | 74.920 | 1.00 | 43.64 | SOLV |

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Figure 16-49

| | | | | | | | | | | |
|--------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| HETATM | 3169 | OH2 | WAT | 183 | 10.441 | 42.659 | 62.744 | 1.00 | 34.51 | SOLV |
| HETATM | 3170 | OH2 | WAT | 184 | 2.095 | 34.482 | 65.810 | 1.00 | 36.49 | SOLV |
| HETATM | 3171 | OH2 | WAT | 185 | 45.749 | 18.286 | 51.615 | 1.00 | 28.19 | SOLV |
| HETATM | 3172 | OH2 | WAT | 186 | 25.771 | 38.332 | 76.707 | 1.00 | 45.53 | SOLV |
| HETATM | 3173 | OH2 | WAT | 187 | 7.228 | 40.382 | 57.542 | 1.00 | 48.91 | SOLV |
| HETATM | 3174 | OH2 | WAT | 188 | 42.972 | 52.824 | 67.739 | 1.00 | 39.99 | SOLV |
| HETATM | 3175 | OH2 | WAT | 189 | 20.137 | 13.189 | 73.277 | 1.00 | 44.91 | SOLV |
| HETATM | 3176 | OH2 | WAT | 190 | 48.945 | 19.193 | 47.581 | 1.00 | 52.88 | SOLV |
| HETATM | 3177 | OH2 | WAT | 191 | 14.549 | 34.547 | 47.665 | 1.00 | 49.15 | SOLV |
| HETATM | 3178 | OH2 | WAT | 192 | 31.765 | 20.567 | 26.536 | 1.00 | 42.23 | SOLV |
| HETATM | 3179 | OH2 | WAT | 193 | 9.784 | 39.303 | 74.222 | 1.00 | 32.10 | SOLV |
| HETATM | 3180 | OH2 | WAT | 194 | 28.865 | 12.481 | 52.375 | 1.00 | 50.98 | SOLV |
| HETATM | 3181 | OH2 | WAT | 195 | 24.030 | 12.804 | 70.409 | 1.00 | 52.43 | SOLV |
| HETATM | 3182 | OH2 | WAT | 196 | 47.209 | 39.536 | 50.698 | 1.00 | 43.03 | SOLV |
| HETATM | 3183 | OH2 | WAT | 197 | 35.618 | 18.114 | 27.306 | 1.00 | 41.11 | SOLV |
| HETATM | 3184 | OH2 | WAT | 198 | 23.625 | 48.145 | 43.853 | 1.00 | 48.20 | SOLV |
| HETATM | 3185 | OH2 | WAT | 199 | 37.090 | 59.044 | 54.185 | 1.00 | 34.99 | SOLV |
| HETATM | 3186 | OH2 | WAT | 200 | 34.478 | 12.208 | 59.080 | 1.00 | 36.58 | SOLV |
| HETATM | 3187 | OH2 | WAT | 201 | 22.142 | 29.583 | 76.228 | 1.00 | 33.95 | SOLV |
| HETATM | 3188 | OH2 | WAT | 202 | 13.608 | 42.619 | 53.973 | 1.00 | 40.44 | SOLV |
| HETATM | 3189 | OH2 | WAT | 203 | 42.647 | 18.701 | 72.526 | 1.00 | 55.64 | SOLV |
| HETATM | 3190 | OH2 | WAT | 204 | 37.005 | 35.993 | 77.480 | 1.00 | 34.82 | SOLV |
| HETATM | 3191 | OH2 | WAT | 205 | 34.154 | 20.512 | 33.327 | 1.00 | 31.00 | SOLV |
| HETATM | 3192 | OH2 | WAT | 206 | 37.264 | 57.546 | 47.642 | 1.00 | 49.58 | SOLV |
| HETATM | 3193 | OH2 | WAT | 207 | 17.924 | 35.195 | 79.003 | 1.00 | 38.45 | SOLV |
| HETATM | 3194 | OH2 | WAT | 208 | 51.172 | 31.581 | 62.378 | 1.00 | 35.37 | SOLV |
| HETATM | 3195 | OH2 | WAT | 209 | 50.503 | 36.726 | 79.224 | 1.00 | 39.95 | SOLV |
| HETATM | 3196 | OH2 | WAT | 210 | 18.382 | 13.162 | 63.852 | 1.00 | 52.08 | SOLV |
| HETATM | 3197 | OH2 | WAT | 211 | 27.245 | 8.351 | 55.199 | 1.00 | 39.12 | SOLV |
| HETATM | 3198 | OH2 | WAT | 212 | 18.354 | 13.545 | 59.540 | 1.00 | 30.15 | SOLV |
| HETATM | 3199 | OH2 | WAT | 213 | 49.088 | 51.744 | 63.388 | 1.00 | 36.69 | SOLV |
| HETATM | 3200 | OH2 | WAT | 214 | 23.251 | 33.160 | 50.871 | 1.00 | 42.11 | SOLV |
| HETATM | 3201 | OH2 | WAT | 215 | 12.989 | 35.073 | 50.651 | 1.00 | 38.63 | SOLV |
| HETATM | 3202 | OH2 | WAT | 216 | 24.414 | 44.460 | 43.239 | 1.00 | 37.93 | SOLV |
| HETATM | 3203 | OH2 | WAT | 217 | 24.690 | 47.590 | 73.117 | 1.00 | 34.17 | SOLV |
| HETATM | 3204 | OH2 | WAT | 218 | 19.844 | 17.949 | 81.360 | 1.00 | 40.74 | SOLV |
| HETATM | 3205 | OH2 | WAT | 219 | 40.169 | 27.215 | 74.247 | 1.00 | 37.83 | SOLV |
| HETATM | 3206 | OH2 | WAT | 220 | 38.737 | 39.516 | 73.171 | 1.00 | 49.20 | SOLV |
| HETATM | 3207 | OH2 | WAT | 221 | 50.628 | 21.408 | 46.879 | 1.00 | 45.57 | SOLV |
| HETATM | 3208 | OH2 | WAT | 222 | 35.436 | 43.288 | 75.660 | 1.00 | 37.33 | SOLV |
| HETATM | 3209 | OH2 | WAT | 223 | 34.390 | 16.963 | 55.285 | 1.00 | 35.10 | SOLV |
| HETATM | 3210 | OH2 | WAT | 224 | 21.800 | 35.454 | 34.475 | 1.00 | 46.29 | SOLV |
| HETATM | 3211 | OH2 | WAT | 225 | 15.751 | 40.989 | 46.787 | 1.00 | 62.75 | SOLV |
| HETATM | 3212 | OH2 | WAT | 226 | 23.844 | 48.662 | 66.295 | 1.00 | 38.35 | SOLV |
| HETATM | 3213 | OH2 | WAT | 227 | 47.225 | 20.562 | 55.117 | 1.00 | 49.99 | SOLV |
| HETATM | 3214 | OH2 | WAT | 228 | 23.426 | 19.272 | 50.565 | 1.00 | 30.07 | SOLV |

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Figure 17-1

| | | | | Residue # | X | Y | Z | OCC. | B | Segment ID | |
|------|----|-----|-----|-----------|----|--------|--------|--------|------|------------|---|
| ATOM | 1 | CB | ALA | A | 2 | 43.739 | 36.862 | 75.052 | 1.00 | 64.01 | 6 |
| ATOM | 2 | C | ALA | A | 2 | 44.405 | 38.106 | 72.971 | 1.00 | 60.02 | 6 |
| ATOM | 3 | O | ALA | A | 2 | 43.251 | 38.536 | 72.908 | 1.00 | 57.94 | 8 |
| ATOM | 4 | N | ALA | A | 2 | 46.142 | 37.179 | 74.497 | 1.00 | 62.88 | 7 |
| ATOM | 5 | CA | ALA | A | 2 | 44.776 | 36.966 | 73.923 | 1.00 | 63.02 | 6 |
| ATOM | 6 | N | LYS | A | 3 | 45.398 | 38.588 | 72.233 | 1.00 | 55.40 | 7 |
| ATOM | 7 | CA | LYS | A | 3 | 45.196 | 39.671 | 71.287 | 1.00 | 53.02 | 6 |
| ATOM | 8 | CB | LYS | A | 3 | 46.443 | 39.830 | 70.421 | 1.00 | 53.11 | 6 |
| ATOM | 9 | CG | LYS | A | 3 | 47.703 | 40.093 | 71.217 | 1.00 | 57.36 | 6 |
| ATOM | 10 | CD | LYS | A | 3 | 48.941 | 39.976 | 70.349 | 1.00 | 60.94 | 6 |
| ATOM | 11 | CE | LYS | A | 3 | 48.909 | 40.957 | 69.196 | 1.00 | 63.48 | 6 |
| ATOM | 12 | NZ | LYS | A | 3 | 50.075 | 40.765 | 68.294 | 1.00 | 66.87 | 7 |
| ATOM | 13 | C | LYS | A | 3 | 43.986 | 39.401 | 70.399 | 1.00 | 50.49 | 6 |
| ATOM | 14 | O | LYS | A | 3 | 43.691 | 38.255 | 70.063 | 1.00 | 52.50 | 8 |
| ATOM | 15 | N | VAL | A | 4 | 43.281 | 40.464 | 70.034 | 1.00 | 45.96 | 7 |
| ATOM | 16 | CA | VAL | A | 4 | 42.122 | 40.352 | 69.167 | 1.00 | 41.16 | 6 |
| ATOM | 17 | CB | VAL | A | 4 | 40.983 | 41.272 | 69.638 | 1.00 | 41.53 | 6 |
| ATOM | 18 | CG1 | VAL | A | 4 | 39.734 | 41.028 | 68.797 | 1.00 | 40.07 | 6 |
| ATOM | 19 | CG2 | VAL | A | 4 | 40.705 | 41.033 | 71.115 | 1.00 | 38.31 | 6 |
| ATOM | 20 | C | VAL | A | 4 | 42.619 | 40.796 | 67.796 | 1.00 | 39.96 | 6 |
| ATOM | 21 | O | VAL | A | 4 | 43.123 | 41.914 | 67.645 | 1.00 | 39.15 | 8 |
| ATOM | 22 | N | LYS | A | 5 | 42.486 | 39.916 | 66.807 | 1.00 | 36.24 | 7 |
| ATOM | 23 | CA | LYS | A | 5 | 42.956 | 40.186 | 65.449 | 1.00 | 35.66 | 6 |
| ATOM | 24 | CB | LYS | A | 5 | 43.930 | 39.088 | 65.024 | 1.00 | 37.33 | 6 |
| ATOM | 25 | CG | LYS | A | 5 | 45.197 | 38.978 | 65.860 | 1.00 | 38.24 | 6 |
| ATOM | 26 | CD | LYS | A | 5 | 46.113 | 40.179 | 65.659 | 1.00 | 35.41 | 6 |
| ATOM | 27 | CE | LYS | A | 5 | 47.436 | 39.957 | 66.369 | 1.00 | 37.46 | 6 |
| ATOM | 28 | NZ | LYS | A | 5 | 48.345 | 41.121 | 66.245 | 1.00 | 35.63 | 7 |
| ATOM | 29 | C | LYS | A | 5 | 41.840 | 40.254 | 64.415 | 1.00 | 34.40 | 6 |
| ATOM | 30 | O | LYS | A | 5 | 40.788 | 39.641 | 64.588 | 1.00 | 33.92 | 8 |
| ATOM | 31 | N | LEU | A | 6 | 42.082 | 40.983 | 63.329 | 1.00 | 32.52 | 7 |
| ATOM | 32 | CA | LEU | A | 6 | 41.097 | 41.094 | 62.253 | 1.00 | 33.64 | 6 |
| ATOM | 33 | CB | LEU | A | 6 | 40.589 | 42.532 | 62.114 | 1.00 | 31.83 | 6 |
| ATOM | 34 | CG | LEU | A | 6 | 39.346 | 42.823 | 61.248 | 1.00 | 32.93 | 6 |
| ATOM | 35 | CD1 | LEU | A | 6 | 39.356 | 44.295 | 60.899 | 1.00 | 28.95 | 6 |
| ATOM | 36 | CD2 | LEU | A | 6 | 39.336 | 42.031 | 59.964 | 1.00 | 32.87 | 6 |
| ATOM | 37 | C | LEU | A | 6 | 41.802 | 40.721 | 60.955 | 1.00 | 35.09 | 6 |
| ATOM | 38 | O | LEU | A | 6 | 42.631 | 41.491 | 60.468 | 1.00 | 36.93 | 8 |
| ATOM | 39 | N | ILE | A | 7 | 41.494 | 39.561 | 60.382 | 1.00 | 35.52 | 7 |
| ATOM | 40 | CA | ILE | A | 7 | 42.145 | 39.199 | 59.129 | 1.00 | 35.14 | 6 |
| ATOM | 41 | CB | ILE | A | 7 | 42.062 | 37.711 | 58.850 | 1.00 | 33.68 | 6 |
| ATOM | 42 | CG2 | ILE | A | 7 | 42.731 | 37.409 | 57.517 | 1.00 | 32.87 | 6 |
| ATOM | 43 | CG1 | ILE | A | 7 | 42.746 | 36.941 | 59.975 | 1.00 | 33.32 | 6 |
| ATOM | 44 | CD1 | ILE | A | 7 | 42.744 | 35.451 | 59.755 | 1.00 | 35.09 | 6 |
| ATOM | 45 | C | ILE | A | 7 | 41.487 | 39.935 | 57.971 | 1.00 | 37.13 | 6 |
| ATOM | 46 | O | ILE | A | 7 | 40.258 | 39.933 | 57.855 | 1.00 | 35.21 | 8 |
| ATOM | 47 | N | GLY | A | 8 | 42.304 | 40.563 | 57.124 | 1.00 | 37.25 | 7 |
| ATOM | 48 | CA | GLY | A | 8 | 41.771 | 41.305 | 55.994 | 1.00 | 38.69 | 6 |
| ATOM | 49 | C | GLY | A | 8 | 42.809 | 41.939 | 55.079 | 1.00 | 39.73 | 6 |
| ATOM | 50 | O | GLY | A | 8 | 44.015 | 41.827 | 55.321 | 1.00 | 39.21 | 8 |
| ATOM | 51 | N | THR | A | 9 | 42.335 | 42.622 | 54.033 | 1.00 | 39.41 | 7 |
| ATOM | 52 | CA | THR | A | 9 | 43.212 | 43.268 | 53.057 | 1.00 | 38.69 | 6 |
| ATOM | 53 | CB | THR | A | 9 | 44.132 | 42.210 | 52.390 | 1.00 | 37.27 | 6 |
| ATOM | 54 | OG1 | THR | A | 9 | 44.754 | 42.771 | 51.230 | 1.00 | 36.82 | 8 |
| ATOM | 55 | CG2 | THR | A | 9 | 43.332 | 40.972 | 52.001 | 1.00 | 38.59 | 6 |
| ATOM | 56 | C | THR | A | 9 | 42.447 | 44.045 | 51.970 | 1.00 | 38.60 | 6 |
| ATOM | 57 | O | THR | A | 9 | 41.434 | 43.569 | 51.452 | 1.00 | 37.30 | 8 |
| ATOM | 58 | N | LEU | A | 10 | 42.939 | 45.238 | 51.628 | 1.00 | 38.14 | 7 |
| ATOM | 59 | CA | LEU | A | 10 | 42.304 | 46.077 | 50.609 | 1.00 | 39.39 | 6 |
| ATOM | 60 | CB | LEU | A | 10 | 43.026 | 47.418 | 50.456 | 1.00 | 38.98 | 6 |
| ATOM | 61 | CG | LEU | A | 10 | 42.836 | 48.506 | 51.510 | 1.00 | 39.68 | 6 |
| ATOM | 62 | CD1 | LEU | A | 10 | 41.343 | 48.830 | 51.594 | 1.00 | 40.22 | 6 |
| ATOM | 63 | CD2 | LEU | A | 10 | 43.382 | 48.057 | 52.857 | 1.00 | 40.11 | 6 |
| ATOM | 64 | C | LEU | A | 10 | 42.238 | 45.432 | 49.239 | 1.00 | 41.66 | 6 |
| ATOM | 65 | O | LEU | A | 10 | 41.462 | 45.863 | 48.381 | 1.00 | 42.08 | 8 |
| ATOM | 66 | N | ASP | A | 11 | 43.052 | 44.408 | 49.025 | 1.00 | 43.51 | 7 |

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Figure 17-2

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 67 | CA | ASP | A | 11 | 43.071 | 43.731 | 47.737 | 1.00 | 47.27 | 6 |
| ATOM | 68 | CB | ASP | A | 11 | 44.250 | 42.765 | 47.694 | 1.00 | 51.03 | 6 |
| ATOM | 69 | CG | ASP | A | 11 | 45.579 | 43.479 | 47.858 | 1.00 | 54.10 | 6 |
| ATOM | 70 | OD1 | ASP | A | 11 | 45.944 | 44.282 | 46.975 | 1.00 | 55.93 | 8 |
| ATOM | 71 | OD2 | ASP | A | 11 | 46.255 | 43.251 | 48.879 | 1.00 | 57.79 | 8 |
| ATOM | 72 | C | ASP | A | 11 | 41.756 | 43.016 | 47.423 | 1.00 | 46.36 | 6 |
| ATOM | 73 | O | ASP | A | 11 | 41.472 | 42.702 | 46.266 | 1.00 | 43.49 | 8 |
| ATOM | 74 | N | TYR | A | 12 | 40.954 | 42.767 | 48.456 | 1.00 | 46.80 | 7 |
| ATOM | 75 | CA | TYR | A | 12 | 39.654 | 42.116 | 48.284 | 1.00 | 45.92 | 6 |
| ATOM | 76 | CB | TYR | A | 12 | 38.953 | 41.942 | 49.638 | 1.00 | 41.38 | 6 |
| ATOM | 77 | CG | TYR | A | 12 | 39.358 | 40.697 | 50.390 | 1.00 | 38.82 | 6 |
| ATOM | 78 | CD1 | TYR | A | 12 | 39.531 | 40.720 | 51.775 | 1.00 | 37.95 | 6 |
| ATOM | 79 | CE1 | TYR | A | 12 | 39.869 | 39.560 | 52.476 | 1.00 | 36.18 | 6 |
| ATOM | 80 | CD2 | TYR | A | 12 | 39.533 | 39.479 | 49.721 | 1.00 | 37.69 | 6 |
| ATOM | 81 | CE2 | TYR | A | 12 | 39.868 | 38.316 | 50.415 | 1.00 | 35.83 | 6 |
| ATOM | 82 | CZ | TYR | A | 12 | 40.032 | 38.365 | 51.787 | 1.00 | 34.10 | 6 |
| ATOM | 83 | OH | TYR | A | 12 | 40.339 | 37.216 | 52.470 | 1.00 | 36.31 | 8 |
| ATOM | 84 | C | TYR | A | 12 | 38.786 | 42.966 | 47.378 | 1.00 | 46.56 | 6 |
| ATOM | 85 | O | TYR | A | 12 | 37.821 | 42.476 | 46.791 | 1.00 | 47.38 | 8 |
| ATOM | 86 | N | GLY | A | 13 | 39.138 | 44.247 | 47.278 | 1.00 | 47.28 | 7 |
| ATOM | 87 | CA | GLY | A | 13 | 38.385 | 45.164 | 46.442 | 1.00 | 46.53 | 6 |
| ATOM | 88 | C | GLY | A | 13 | 38.650 | 44.934 | 44.968 | 1.00 | 45.60 | 6 |
| ATOM | 89 | O | GLY | A | 13 | 37.895 | 45.401 | 44.117 | 1.00 | 43.68 | 8 |
| ATOM | 90 | N | LYS | A | 14 | 39.725 | 44.210 | 44.672 | 1.00 | 46.52 | 7 |
| ATOM | 91 | CA | LYS | A | 14 | 40.112 | 43.908 | 43.296 | 1.00 | 47.28 | 6 |
| ATOM | 92 | CB | LYS | A | 14 | 41.629 | 43.748 | 43.201 | 1.00 | 50.22 | 6 |
| ATOM | 93 | CG | LYS | A | 14 | 42.396 | 45.044 | 43.307 | 1.00 | 57.12 | 6 |
| ATOM | 94 | CD | LYS | A | 14 | 42.038 | 46.004 | 42.161 | 1.00 | 63.60 | 6 |
| ATOM | 95 | CE | LYS | A | 14 | 42.349 | 45.422 | 40.768 | 1.00 | 66.65 | 6 |
| ATOM | 96 | NZ | LYS | A | 14 | 41.529 | 44.220 | 40.387 | 1.00 | 67.70 | 7 |
| ATOM | 97 | C | LYS | A | 14 | 39.460 | 42.643 | 42.769 | 1.00 | 44.18 | 6 |
| ATOM | 98 | O | LYS | A | 14 | 39.564 | 42.325 | 41.585 | 1.00 | 40.33 | 8 |
| ATOM | 99 | N | TYR | A | 15 | 38.790 | 41.926 | 43.661 | 1.00 | 43.25 | 7 |
| ATOM | 100 | CA | TYR | A | 15 | 38.145 | 40.665 | 43.317 | 1.00 | 43.18 | 6 |
| ATOM | 101 | CB | TYR | A | 15 | 38.789 | 39.547 | 44.142 | 1.00 | 36.88 | 6 |
| ATOM | 102 | CG | TYR | A | 15 | 40.302 | 39.560 | 44.053 | 1.00 | 32.96 | 6 |
| ATOM | 103 | CD1 | TYR | A | 15 | 41.084 | 39.107 | 45.108 | 1.00 | 30.90 | 6 |
| ATOM | 104 | CE1 | TYR | A | 15 | 42.476 | 39.144 | 45.035 | 1.00 | 30.94 | 6 |
| ATOM | 105 | CD2 | TYR | A | 15 | 40.952 | 40.049 | 42.912 | 1.00 | 33.01 | 6 |
| ATOM | 106 | CE2 | TYR | A | 15 | 42.341 | 40.092 | 42.826 | 1.00 | 29.68 | 6 |
| ATOM | 107 | CZ | TYR | A | 15 | 43.098 | 39.639 | 43.890 | 1.00 | 30.99 | 6 |
| ATOM | 108 | OH | TYR | A | 15 | 44.471 | 39.673 | 43.809 | 1.00 | 28.02 | 8 |
| ATOM | 109 | C | TYR | A | 15 | 36.661 | 40.778 | 43.621 | 1.00 | 45.56 | 6 |
| ATOM | 110 | O | TYR | A | 15 | 36.149 | 40.153 | 44.552 | 1.00 | 45.22 | 8 |
| ATOM | 111 | N | ARG | A | 16 | 35.981 | 41.599 | 42.830 | 1.00 | 48.81 | 7 |
| ATOM | 112 | CA | ARG | A | 16 | 34.553 | 41.819 | 42.999 | 1.00 | 53.22 | 6 |
| ATOM | 113 | CB | ARG | A | 16 | 34.193 | 43.263 | 42.654 | 1.00 | 57.11 | 5 |
| ATOM | 114 | CG | ARG | A | 16 | 34.852 | 44.330 | 43.490 | 1.00 | 61.66 | 6 |
| ATOM | 115 | CD | ARG | A | 16 | 34.280 | 44.408 | 44.886 | 1.00 | 67.04 | 6 |
| ATOM | 116 | NE | ARG | A | 16 | 34.798 | 45.590 | 45.569 | 1.00 | 73.59 | 7 |
| ATOM | 117 | CZ | ARG | A | 16 | 34.612 | 46.837 | 45.141 | 1.00 | 75.03 | 6 |
| ATOM | 118 | NH1 | ARG | A | 16 | 33.917 | 47.065 | 44.033 | 1.00 | 73.03 | 7 |
| ATOM | 119 | NH2 | ARG | A | 16 | 35.142 | 47.856 | 45.808 | 1.00 | 75.79 | 7 |
| ATOM | 120 | C | ARG | A | 16 | 33.757 | 40.903 | 42.080 | 1.00 | 51.79 | 6 |
| ATOM | 121 | O | ARG | A | 16 | 34.192 | 40.593 | 40.970 | 1.00 | 50.89 | 8 |
| ATOM | 122 | N | TYR | A | 17 | 32.596 | 40.463 | 42.552 | 1.00 | 50.19 | 7 |
| ATOM | 123 | CA | TYR | A | 17 | 31.737 | 39.634 | 41.733 | 1.00 | 49.60 | 6 |
| ATOM | 124 | CB | TYR | A | 17 | 30.534 | 39.119 | 42.528 | 1.00 | 45.80 | 6 |
| ATOM | 125 | CG | TYR | A | 17 | 30.803 | 37.894 | 43.365 | 1.00 | 42.01 | 6 |
| ATOM | 126 | CD1 | TYR | A | 17 | 31.689 | 37.932 | 44.438 | 1.00 | 42.45 | 6 |
| ATOM | 127 | CE1 | TYR | A | 17 | 31.960 | 36.780 | 45.193 | 1.00 | 43.36 | 6 |
| ATOM | 128 | CD2 | TYR | A | 17 | 30.185 | 36.680 | 43.062 | 1.00 | 39.89 | 6 |
| ATOM | 129 | CE2 | TYR | A | 17 | 30.443 | 35.526 | 43.803 | 1.00 | 40.56 | 6 |
| ATOM | 130 | CZ | TYR | A | 17 | 31.333 | 35.578 | 44.869 | 1.00 | 41.98 | 6 |
| ATOM | 131 | OH | TYR | A | 17 | 31.600 | 34.438 | 45.598 | 1.00 | 34.66 | 8 |
| ATOM | 132 | C | TYR | A | 17 | 31.245 | 40.547 | 40.622 | 1.00 | 51.88 | 6 |

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Figure 17-3

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 133 | O | TYR | A | 17 | 31.332 | 41.772 | 40.726 | 1.00 | 47.86 | 8 |
| ATOM | 134 | N | PRO | A | 18 | 30.730 | 39.964 | 39.534 | 1.00 | 54.38 | 7 |
| ATOM | 135 | CD | PRO | A | 18 | 30.548 | 38.545 | 39.190 | 1.00 | 54.21 | 6 |
| ATOM | 136 | CA | PRO | A | 18 | 30.243 | 40.809 | 38.449 | 1.00 | 56.43 | 6 |
| ATOM | 137 | CB | PRO | A | 18 | 29.601 | 39.792 | 37.496 | 1.00 | 56.84 | 6 |
| ATOM | 138 | CG | PRO | A | 18 | 29.260 | 38.613 | 38.426 | 1.00 | 56.46 | 6 |
| ATOM | 139 | C | PRO | A | 18 | 29.273 | 41.891 | 38.932 | 1.00 | 58.74 | 6 |
| ATOM | 140 | O | PRO | A | 18 | 28.791 | 41.861 | 40.066 | 1.00 | 55.72 | 8 |
| ATOM | 141 | N | LYS | A | 19 | 29.017 | 42.851 | 38.052 | 1.00 | 62.10 | 7 |
| ATOM | 142 | CA | LYS | A | 19 | 28.127 | 43.973 | 38.314 | 1.00 | 64.85 | 6 |
| ATOM | 143 | CB | LYS | A | 19 | 27.972 | 44.781 | 37.022 | 1.00 | 69.74 | 6 |
| ATOM | 144 | CG | LYS | A | 19 | 28.008 | 43.925 | 35.740 | 1.00 | 74.99 | 6 |
| ATOM | 145 | CD | LYS | A | 19 | 26.895 | 42.881 | 35.668 | 1.00 | 78.18 | 6 |
| ATOM | 146 | CE | LYS | A | 19 | 26.981 | 42.010 | 34.420 | 1.00 | 80.24 | 6 |
| ATOM | 147 | NZ | LYS | A | 19 | 25.867 | 41.010 | 34.361 | 1.00 | 81.13 | 7 |
| ATOM | 148 | C | LYS | A | 19 | 26.750 | 43.619 | 38.869 | 1.00 | 64.77 | 6 |
| ATOM | 149 | O | LYS | A | 19 | 26.414 | 43.961 | 40.001 | 1.00 | 66.50 | 8 |
| ATOM | 150 | N | ASN | A | 20 | 25.957 | 42.933 | 38.062 | 1.00 | 63.75 | 7 |
| ATOM | 151 | CA | ASN | A | 20 | 24.612 | 42.556 | 38.439 | 1.00 | 62.96 | 6 |
| ATOM | 152 | CB | ASN | A | 20 | 23.870 | 42.031 | 37.208 | 1.00 | 67.42 | 6 |
| ATOM | 153 | CG | ASN | A | 20 | 22.392 | 41.833 | 37.459 | 1.00 | 72.29 | 6 |
| ATOM | 154 | OD1 | ASN | A | 20 | 21.666 | 42.785 | 37.772 | 1.00 | 75.25 | 8 |
| ATOM | 155 | ND2 | ASN | A | 20 | 21.931 | 40.594 | 37.322 | 1.00 | 74.38 | 7 |
| ATOM | 156 | C | ASN | A | 20 | 24.602 | 41.512 | 39.547 | 1.00 | 61.30 | 6 |
| ATOM | 157 | O | ASN | A | 20 | 23.629 | 40.773 | 39.698 | 1.00 | 61.49 | 8 |
| ATOM | 158 | N | HIS | A | 21 | 25.681 | 41.444 | 40.321 | 1.00 | 57.30 | 7 |
| ATOM | 159 | CA | HIS | A | 21 | 25.755 | 40.480 | 41.418 | 1.00 | 54.68 | 6 |
| ATOM | 160 | CB | HIS | A | 21 | 27.071 | 39.700 | 41.373 | 1.00 | 52.63 | 6 |
| ATOM | 161 | CG | HIS | A | 21 | 27.058 | 38.449 | 42.195 | 1.00 | 49.39 | 6 |
| ATOM | 162 | CD2 | HIS | A | 21 | 27.336 | 38.236 | 43.503 | 1.00 | 49.39 | 6 |
| ATOM | 163 | ND1 | HIS | A | 21 | 26.664 | 37.229 | 41.686 | 1.00 | 48.27 | 7 |
| ATOM | 164 | CE1 | HIS | A | 21 | 26.704 | 36.320 | 42.643 | 1.00 | 48.16 | 6 |
| ATOM | 165 | NE2 | HIS | A | 21 | 27.108 | 36.905 | 43.757 | 1.00 | 47.33 | 7 |
| ATOM | 166 | C | HIS | A | 21 | 25.664 | 41.215 | 42.760 | 1.00 | 52.89 | 6 |
| ATOM | 167 | O | HIS | A | 21 | 26.295 | 42.256 | 42.947 | 1.00 | 52.52 | 8 |
| ATOM | 168 | N | PRO | A | 22 | 24.880 | 40.679 | 43.713 | 1.00 | 50.81 | 7 |
| ATOM | 169 | CD | PRO | A | 22 | 24.076 | 39.444 | 43.661 | 1.00 | 48.50 | 6 |
| ATOM | 170 | CA | PRO | A | 22 | 24.734 | 41.310 | 45.029 | 1.00 | 48.02 | 6 |
| ATOM | 171 | CB | PRO | A | 22 | 23.860 | 40.308 | 45.783 | 1.00 | 47.45 | 6 |
| ATOM | 172 | CG | PRO | A | 22 | 22.990 | 39.754 | 44.667 | 1.00 | 47.76 | 6 |
| ATOM | 173 | C | PRO | A | 22 | 26.074 | 41.558 | 45.727 | 1.00 | 46.48 | 6 |
| ATOM | 174 | O | PRO | A | 22 | 26.164 | 42.405 | 46.615 | 1.00 | 45.69 | 8 |
| ATOM | 175 | N | LEU | A | 23 | 27.107 | 40.816 | 45.318 | 1.00 | 44.97 | 7 |
| ATOM | 176 | CA | LEU | A | 23 | 28.441 | 40.949 | 45.906 | 1.00 | 41.31 | 6 |
| ATOM | 177 | CB | LEU | A | 23 | 29.076 | 39.569 | 46.131 | 1.00 | 39.22 | 6 |
| ATOM | 178 | CG | LEU | A | 23 | 28.264 | 38.561 | 46.953 | 1.00 | 37.71 | 6 |
| ATOM | 179 | CD1 | LEU | A | 23 | 29.075 | 37.288 | 47.157 | 1.00 | 35.07 | 6 |
| ATOM | 180 | CD2 | LEU | A | 23 | 27.896 | 39.165 | 48.292 | 1.00 | 36.90 | 6 |
| ATOM | 181 | C | LEU | A | 23 | 29.334 | 41.789 | 45.003 | 1.00 | 40.14 | 6 |
| ATOM | 182 | O | LEU | A | 23 | 30.556 | 41.614 | 44.951 | 1.00 | 39.00 | 8 |
| ATOM | 183 | N | LYS | A | 24 | 28.706 | 42.705 | 44.284 | 1.00 | 39.67 | 7 |
| ATOM | 184 | CA | LYS | A | 24 | 29.430 | 43.590 | 43.398 | 1.00 | 42.88 | 6 |
| ATOM | 185 | CB | LYS | A | 24 | 28.480 | 44.120 | 42.323 | 1.00 | 40.24 | 6 |
| ATOM | 186 | CG | LYS | A | 24 | 28.949 | 45.362 | 41.610 | 1.00 | 44.08 | 6 |
| ATOM | 187 | CD | LYS | A | 24 | 28.247 | 46.600 | 42.166 | 1.00 | 44.47 | 6 |
| ATOM | 188 | CE | LYS | A | 24 | 26.732 | 46.492 | 41.968 | 1.00 | 43.23 | 6 |
| ATOM | 189 | NZ | LYS | A | 24 | 25.989 | 47.717 | 42.362 | 1.00 | 39.79 | 7 |
| ATOM | 190 | C | LYS | A | 24 | 30.031 | 44.723 | 44.217 | 1.00 | 43.70 | 6 |
| ATOM | 191 | O | LYS | A | 24 | 31.027 | 45.332 | 43.817 | 1.00 | 47.22 | 8 |
| ATOM | 192 | N | ILE | A | 25 | 29.431 | 44.976 | 45.378 | 1.00 | 42.27 | 7 |
| ATOM | 193 | CA | ILE | A | 25 | 29.870 | 46.035 | 46.289 | 1.00 | 39.86 | 6 |
| ATOM | 194 | CB | ILE | A | 25 | 28.763 | 46.407 | 47.306 | 1.00 | 37.72 | 6 |
| ATOM | 195 | CG2 | ILE | A | 25 | 27.539 | 46.953 | 46.580 | 1.00 | 39.67 | 6 |
| ATOM | 196 | CG1 | ILE | A | 25 | 28.410 | 45.168 | 48.145 | 1.00 | 35.25 | 6 |
| ATOM | 197 | CD1 | ILE | A | 25 | 27.301 | 45.368 | 49.151 | 1.00 | 31.74 | 6 |
| ATOM | 198 | C | ILE | A | 25 | 31.078 | 45.625 | 47.112 | 1.00 | 40.23 | 6 |

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Figure 17-4

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 199 | O | ILE | A | 25 | 31.419 | 44.441 | 47.198 | 1.00 | 38.90 | 8 |
| ATOM | 200 | N | PRO | A | 26 | 31.762 | 46.616 | 47.709 | 1.00 | 40.18 | 7 |
| ATOM | 201 | CD | PRO | A | 26 | 31.523 | 48.051 | 47.533 | 1.00 | 40.58 | 6 |
| ATOM | 202 | CA | PRO | A | 26 | 32.939 | 46.437 | 48.558 | 1.00 | 38.31 | 6 |
| ATOM | 203 | CB | PRO | A | 26 | 33.478 | 47.860 | 48.688 | 1.00 | 37.14 | 6 |
| ATOM | 204 | CG | PRO | A | 26 | 32.940 | 48.537 | 47.458 | 1.00 | 38.77 | 6 |
| ATOM | 205 | C | PRO | A | 26 | 32.433 | 45.903 | 49.891 | 1.00 | 37.32 | 6 |
| ATOM | 206 | O | PRO | A | 26 | 31.416 | 46.372 | 50.412 | 1.00 | 32.70 | 8 |
| ATOM | 207 | N | ARG | A | 27 | 33.134 | 44.930 | 50.452 | 1.00 | 36.54 | 7 |
| ATOM | 208 | CA | ARG | A | 27 | 32.685 | 44.359 | 51.711 | 1.00 | 37.39 | 6 |
| ATOM | 209 | CB | ARG | A | 27 | 32.116 | 42.952 | 51.455 | 1.00 | 35.29 | 6 |
| ATOM | 210 | CG | ARG | A | 27 | 31.047 | 42.956 | 50.355 | 1.00 | 32.69 | 6 |
| ATOM | 211 | CD | ARG | A | 27 | 30.507 | 41.573 | 49.956 | 1.00 | 33.87 | 6 |
| ATOM | 212 | NE | ARG | A | 27 | 29.757 | 40.909 | 51.021 | 1.00 | 36.16 | 7 |
| ATOM | 213 | CZ | ARG | A | 27 | 30.293 | 40.132 | 51.959 | 1.00 | 37.11 | 6 |
| ATOM | 214 | NH1 | ARG | A | 27 | 31.604 | 39.903 | 51.976 | 1.00 | 34.42 | 7 |
| ATOM | 215 | NH2 | ARG | A | 27 | 29.516 | 39.597 | 52.896 | 1.00 | 33.67 | 7 |
| ATOM | 216 | C | ARG | A | 27 | 33.813 | 44.329 | 52.732 | 1.00 | 36.35 | 6 |
| ATOM | 217 | O | ARG | A | 27 | 33.881 | 45.188 | 53.610 | 1.00 | 35.77 | 8 |
| ATOM | 218 | N | VAL | A | 28 | 34.703 | 43.351 | 52.607 | 1.00 | 34.93 | 7 |
| ATOM | 219 | CA | VAL | A | 28 | 35.810 | 43.230 | 53.537 | 1.00 | 34.00 | 6 |
| ATOM | 220 | CB | VAL | A | 28 | 36.633 | 41.954 | 53.252 | 1.00 | 36.21 | 6 |
| ATOM | 221 | CG1 | VAL | A | 28 | 37.574 | 41.652 | 54.424 | 1.00 | 33.59 | 6 |
| ATOM | 222 | CG2 | VAL | A | 28 | 35.696 | 40.790 | 52.992 | 1.00 | 37.05 | 6 |
| ATOM | 223 | C | VAL | A | 28 | 36.712 | 44.454 | 53.423 | 1.00 | 31.91 | 6 |
| ATOM | 224 | O | VAL | A | 28 | 37.216 | 44.959 | 54.427 | 1.00 | 31.45 | 8 |
| ATOM | 225 | N | SER | A | 29 | 36.908 | 44.936 | 52.199 | 1.00 | 33.12 | 7 |
| ATOM | 226 | CA | SER | A | 29 | 37.751 | 46.111 | 51.967 | 1.00 | 32.03 | 6 |
| ATOM | 227 | CB | SER | A | 29 | 38.205 | 46.181 | 50.499 | 1.00 | 31.77 | 6 |
| ATOM | 228 | OG | SER | A | 29 | 37.113 | 46.223 | 49.600 | 1.00 | 30.80 | 8 |
| ATOM | 229 | C | SER | A | 29 | 37.003 | 47.380 | 52.353 | 1.00 | 30.16 | 6 |
| ATOM | 230 | O | SER | A | 29 | 37.604 | 48.404 | 52.650 | 1.00 | 28.70 | 8 |
| ATOM | 231 | N | LEU | A | 30 | 35.682 | 47.310 | 52.352 | 1.00 | 32.43 | 7 |
| ATOM | 232 | CA | LEU | A | 30 | 34.900 | 48.465 | 52.745 | 1.00 | 34.56 | 6 |
| ATOM | 233 | CB | LEU | A | 30 | 33.463 | 48.358 | 52.221 | 1.00 | 36.44 | 6 |
| ATOM | 234 | CG | LEU | A | 30 | 32.508 | 49.513 | 52.560 | 1.00 | 36.79 | 6 |
| ATOM | 235 | CD1 | LEU | A | 30 | 32.070 | 49.446 | 54.012 | 1.00 | 36.73 | 6 |
| ATOM | 236 | CD2 | LEU | A | 30 | 33.202 | 50.840 | 52.256 | 1.00 | 37.84 | 6 |
| ATOM | 237 | C | LEU | A | 30 | 34.902 | 48.527 | 54.262 | 1.00 | 34.89 | 6 |
| ATOM | 238 | O | LEU | A | 30 | 35.033 | 49.601 | 54.841 | 1.00 | 37.58 | 8 |
| ATOM | 239 | N | LEU | A | 31 | 34.761 | 47.366 | 54.897 | 1.00 | 34.07 | 7 |
| ATOM | 240 | CA | LEU | A | 31 | 34.743 | 47.276 | 56.350 | 1.00 | 34.85 | 6 |
| ATOM | 241 | CB | LEU | A | 31 | 34.768 | 45.808 | 56.791 | 1.00 | 36.37 | 6 |
| ATOM | 242 | CG | LEU | A | 31 | 34.459 | 45.471 | 58.261 | 1.00 | 36.04 | 6 |
| ATOM | 243 | CD1 | LEU | A | 31 | 34.841 | 44.027 | 58.532 | 1.00 | 35.13 | 6 |
| ATOM | 244 | CD2 | LEU | A | 31 | 35.228 | 46.357 | 59.194 | 1.00 | 35.86 | 6 |
| ATOM | 245 | C | LEU | A | 31 | 35.976 | 47.994 | 56.894 | 1.00 | 36.43 | 6 |
| ATOM | 246 | O | LEU | A | 31 | 35.855 | 49.035 | 57.544 | 1.00 | 35.87 | 8 |
| ATOM | 247 | N | LEU | A | 32 | 37.157 | 47.426 | 56.635 | 1.00 | 37.76 | 7 |
| ATOM | 248 | CA | LEU | A | 32 | 38.420 | 48.015 | 57.087 | 1.00 | 36.82 | 6 |
| ATOM | 249 | CB | LEU | A | 32 | 39.611 | 47.318 | 56.418 | 1.00 | 36.37 | 6 |
| ATOM | 250 | CG | LEU | A | 32 | 40.030 | 45.888 | 56.774 | 1.00 | 39.11 | 6 |
| ATOM | 251 | CD1 | LEU | A | 32 | 41.117 | 45.420 | 55.815 | 1.00 | 35.16 | 6 |
| ATOM | 252 | CD2 | LEU | A | 32 | 40.538 | 45.830 | 58.214 | 1.00 | 37.73 | 6 |
| ATOM | 253 | C | LEU | A | 32 | 38.500 | 49.513 | 56.780 | 1.00 | 34.84 | 6 |
| ATOM | 254 | O | LEU | A | 32 | 38.846 | 50.326 | 57.644 | 1.00 | 36.58 | 8 |
| ATOM | 255 | N | ARG | A | 33 | 38.184 | 49.877 | 55.545 | 1.00 | 31.37 | 7 |
| ATOM | 256 | CA | ARG | A | 33 | 38.247 | 51.270 | 55.150 | 1.00 | 32.53 | 6 |
| ATOM | 257 | CB | ARG | A | 33 | 37.927 | 51.398 | 53.662 | 1.00 | 31.52 | 6 |
| ATOM | 258 | CG | ARG | A | 33 | 38.481 | 52.652 | 53.642 | 1.00 | 35.88 | 6 |
| ATOM | 259 | CD | ARG | A | 33 | 38.107 | 52.752 | 51.581 | 1.00 | 43.44 | 6 |
| ATOM | 260 | NE | ARG | A | 33 | 38.521 | 51.583 | 50.811 | 1.00 | 48.37 | 7 |
| ATOM | 261 | CZ | ARG | A | 33 | 38.348 | 51.469 | 49.497 | 1.00 | 52.27 | 6 |
| ATOM | 262 | NH1 | ARG | A | 33 | 37.771 | 52.459 | 48.823 | 1.00 | 51.75 | 7 |
| ATOM | 263 | NH2 | ARG | A | 33 | 38.739 | 50.369 | 48.858 | 1.00 | 51.08 | 7 |
| ATOM | 264 | C | ARG | A | 33 | 37.274 | 52.102 | 55.989 | 1.00 | 32.32 | 6 |

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Figure 17-5

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 265 | O | ARG | A | 33 | 37.471 | 53.299 | 56.196 | 1.00 | 29.23 | 8 |
| ATOM | 266 | N | PHE | A | 34 | 36.231 | 51.445 | 56.484 | 1.00 | 32.58 | 7 |
| ATOM | 267 | CA | PHE | A | 34 | 35.216 | 52.096 | 57.304 | 1.00 | 32.69 | 6 |
| ATOM | 268 | CB | PHE | A | 34 | 33.952 | 51.232 | 57.359 | 1.00 | 31.22 | 6 |
| ATOM | 269 | CG | PHE | A | 34 | 32.838 | 51.825 | 58.183 | 1.00 | 28.74 | 6 |
| ATOM | 270 | CD1 | PHE | A | 34 | 32.085 | 52.888 | 57.700 | 1.00 | 22.76 | 6 |
| ATOM | 271 | CD2 | PHE | A | 34 | 32.551 | 51.322 | 59.456 | 1.00 | 28.09 | 6 |
| ATOM | 272 | CE1 | PHE | A | 34 | 31.061 | 53.441 | 58.472 | 1.00 | 23.70 | 6 |
| ATOM | 273 | CE2 | PHE | A | 34 | 31.524 | 51.873 | 60.235 | 1.00 | 24.59 | 6 |
| ATOM | 274 | CZ | PHE | A | 34 | 30.781 | 52.929 | 59.741 | 1.00 | 21.39 | 6 |
| ATOM | 275 | C | PHE | A | 34 | 35.734 | 52.319 | 58.719 | 1.00 | 33.45 | 6 |
| ATOM | 276 | O | PHE | A | 34 | 35.635 | 53.425 | 59.258 | 1.00 | 35.49 | 8 |
| ATOM | 277 | N | LYS | A | 35 | 36.276 | 51.264 | 59.323 | 1.00 | 34.52 | 7 |
| ATOM | 278 | CA | LYS | A | 35 | 36.805 | 51.360 | 60.678 | 1.00 | 36.51 | 6 |
| ATOM | 279 | CB | LYS | A | 35 | 37.118 | 49.977 | 61.235 | 1.00 | 36.47 | 6 |
| ATOM | 280 | CG | LYS | A | 35 | 35.912 | 49.074 | 61.343 | 1.00 | 40.81 | 6 |
| ATOM | 281 | CD | LYS | A | 35 | 36.246 | 47.801 | 62.090 | 1.00 | 44.10 | 6 |
| ATOM | 282 | CE | LYS | A | 35 | 37.347 | 47.029 | 61.402 | 1.00 | 47.46 | 6 |
| ATOM | 283 | NZ | LYS | A | 35 | 38.601 | 47.823 | 61.276 | 1.00 | 53.53 | 7 |
| ATOM | 284 | C | LYS | A | 35 | 38.054 | 52.222 | 60.735 | 1.00 | 36.61 | 6 |
| ATOM | 285 | O | LYS | A | 35 | 38.352 | 52.824 | 61.766 | 1.00 | 36.78 | 8 |
| ATOM | 286 | N | ASP | A | 36 | 38.794 | 52.267 | 59.635 | 1.00 | 36.27 | 7 |
| ATOM | 287 | CA | ASP | A | 36 | 39.980 | 53.090 | 59.592 | 1.00 | 39.71 | 6 |
| ATOM | 288 | CB | ASP | A | 36 | 40.679 | 52.937 | 58.239 | 1.00 | 44.78 | 6 |
| ATOM | 289 | CG | ASP | A | 36 | 41.863 | 53.892 | 58.075 | 1.00 | 47.10 | 6 |
| ATOM | 290 | OD1 | ASP | A | 36 | 42.803 | 53.852 | 58.906 | 1.00 | 44.02 | 8 |
| ATOM | 291 | OD2 | ASP | A | 36 | 41.843 | 54.682 | 57.106 | 1.00 | 48.43 | 8 |
| ATOM | 292 | C | ASP | A | 36 | 39.508 | 54.530 | 59.789 | 1.00 | 39.99 | 6 |
| ATOM | 293 | O | ASP | A | 36 | 40.023 | 55.258 | 60.636 | 1.00 | 40.76 | 8 |
| ATOM | 294 | N | ALA | A | 37 | 38.506 | 54.919 | 59.007 | 1.00 | 38.59 | 7 |
| ATOM | 295 | CA | ALA | A | 37 | 37.939 | 56.258 | 59.066 | 1.00 | 37.14 | 6 |
| ATOM | 296 | CB | ALA | A | 37 | 36.857 | 56.402 | 58.000 | 1.00 | 35.85 | 6 |
| ATOM | 297 | C | ALA | A | 37 | 37.354 | 56.549 | 60.446 | 1.00 | 38.34 | 6 |
| ATOM | 298 | O | ALA | A | 37 | 37.391 | 57.687 | 60.928 | 1.00 | 37.32 | 8 |
| ATOM | 299 | N | MET | A | 38 | 36.809 | 55.518 | 61.079 | 1.00 | 36.19 | 7 |
| ATOM | 300 | CA | MET | A | 38 | 36.213 | 55.674 | 62.397 | 1.00 | 36.80 | 6 |
| ATOM | 301 | CB | MET | A | 38 | 35.141 | 54.598 | 62.606 | 1.00 | 37.38 | 6 |
| ATOM | 302 | CG | MET | A | 38 | 33.938 | 54.717 | 61.673 | 1.00 | 37.60 | 6 |
| ATOM | 303 | SD | MET | A | 38 | 32.887 | 56.165 | 61.999 | 1.00 | 33.61 | 16 |
| ATOM | 304 | CE | MET | A | 38 | 32.398 | 55.824 | 63.680 | 1.00 | 35.60 | 6 |
| ATOM | 305 | C | MET | A | 38 | 37.262 | 55.582 | 63.502 | 1.00 | 35.84 | 6 |
| ATOM | 306 | O | MET | A | 38 | 36.937 | 55.688 | 64.692 | 1.00 | 34.89 | 8 |
| ATOM | 307 | N | ASN | A | 39 | 38.518 | 55.400 | 63.100 | 1.00 | 33.83 | 7 |
| ATOM | 308 | CA | ASN | A | 39 | 39.626 | 55.264 | 64.044 | 1.00 | 34.94 | 6 |
| ATOM | 309 | CB | ASN | A | 39 | 39.897 | 56.582 | 64.775 | 1.00 | 32.48 | 6 |
| ATOM | 310 | CG | ASN | A | 39 | 40.213 | 57.717 | 63.825 | 1.00 | 32.34 | 6 |
| ATOM | 311 | OD1 | ASN | A | 39 | 41.128 | 57.621 | 63.009 | 1.00 | 31.85 | 8 |
| ATOM | 312 | ND2 | ASN | A | 39 | 39.455 | 58.800 | 63.924 | 1.00 | 30.92 | 7 |
| ATOM | 313 | C | ASN | A | 39 | 39.253 | 54.183 | 65.045 | 1.00 | 36.87 | 6 |
| ATOM | 314 | O | ASN | A | 39 | 39.403 | 54.357 | 66.260 | 1.00 | 36.60 | 8 |
| ATOM | 315 | N | LEU | A | 40 | 38.752 | 53.067 | 64.518 | 1.00 | 37.48 | 7 |
| ATOM | 316 | CA | LEU | A | 40 | 38.341 | 51.933 | 65.336 | 1.00 | 39.66 | 6 |
| ATOM | 317 | CB | LEU | A | 40 | 36.863 | 51.622 | 65.086 | 1.00 | 41.35 | 6 |
| ATOM | 318 | CG | LEU | A | 40 | 35.858 | 52.712 | 65.476 | 1.00 | 42.69 | 6 |
| ATOM | 319 | CD1 | LEU | A | 40 | 34.448 | 52.261 | 65.111 | 1.00 | 45.05 | 6 |
| ATOM | 320 | CD2 | LEU | A | 40 | 35.951 | 52.989 | 66.966 | 1.00 | 39.44 | 6 |
| ATOM | 321 | C | LEU | A | 40 | 39.184 | 50.687 | 65.058 | 1.00 | 39.79 | 6 |
| ATOM | 322 | O | LEU | A | 40 | 38.804 | 49.575 | 65.434 | 1.00 | 36.88 | 8 |
| ATOM | 323 | N | ILE | A | 41 | 40.337 | 50.889 | 64.420 | 1.00 | 40.50 | 7 |
| ATOM | 324 | CA | ILE | A | 41 | 41.237 | 49.790 | 64.068 | 1.00 | 41.39 | 6 |
| ATOM | 325 | CB | ILE | A | 41 | 40.780 | 49.141 | 62.724 | 1.00 | 39.24 | 6 |
| ATOM | 326 | CG2 | ILE | A | 41 | 41.017 | 50.103 | 61.564 | 1.00 | 36.97 | 6 |
| ATOM | 327 | CG1 | ILE | A | 41 | 41.513 | 47.824 | 62.482 | 1.00 | 36.76 | 6 |
| ATOM | 328 | CD1 | ILE | A | 41 | 41.085 | 46.715 | 63.403 | 1.00 | 35.59 | 6 |
| ATOM | 329 | C | ILE | A | 41 | 42.684 | 50.295 | 63.913 | 1.00 | 44.37 | 6 |
| ATOM | 330 | O | ILE | A | 41 | 42.927 | 51.328 | 63.277 | 1.00 | 46.01 | 8 |

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Figure 17-6

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 331 | N | ASP | A | 42 | 43.646 | 49.582 | 64.497 | 1.00 | 45.19 | 7 |
| ATOM | 332 | CA | ASP | A | 42 | 45.049 | 49.982 | 64.372 | 1.00 | 45.62 | 6 |
| ATOM | 333 | CB | ASP | A | 42 | 45.716 | 50.090 | 65.742 | 1.00 | 45.17 | 6 |
| ATOM | 334 | CG | ASP | A | 42 | 44.966 | 51.005 | 66.682 | 1.00 | 44.43 | 6 |
| ATOM | 335 | OD1 | ASP | A | 42 | 44.731 | 52.177 | 66.322 | 1.00 | 39.84 | 8 |
| ATOM | 336 | OD2 | ASP | A | 42 | 44.612 | 50.546 | 67.787 | 1.00 | 48.50 | 8 |
| ATOM | 337 | C | ASP | A | 42 | 45.750 | 48.915 | 63.551 | 1.00 | 48.47 | 6 |
| ATOM | 338 | O | ASP | A | 42 | 45.316 | 47.757 | 63.547 | 1.00 | 49.85 | 8 |
| ATOM | 339 | N | GLU | A | 43 | 46.830 | 49.288 | 62.864 | 1.00 | 49.24 | 7 |
| ATOM | 340 | CA | GLU | A | 43 | 47.553 | 48.325 | 62.028 | 1.00 | 50.79 | 6 |
| ATOM | 341 | CB | GLU | A | 43 | 48.820 | 48.956 | 61.431 | 1.00 | 49.90 | 6 |
| ATOM | 342 | CG | GLU | A | 43 | 48.544 | 50.029 | 60.378 | 1.00 | 57.20 | 6 |
| ATOM | 343 | CD | GLU | A | 43 | 49.808 | 50.537 | 59.690 | 1.00 | 59.56 | 6 |
| ATOM | 344 | OE1 | GLU | A | 43 | 50.517 | 49.721 | 59.061 | 1.00 | 65.05 | 8 |
| ATOM | 345 | OE2 | GLU | A | 43 | 50.095 | 51.750 | 59.772 | 1.00 | 57.82 | 8 |
| ATOM | 346 | C | GLU | A | 43 | 47.918 | 47.020 | 62.733 | 1.00 | 49.73 | 6 |
| ATOM | 347 | O | GLU | A | 43 | 47.813 | 45.943 | 62.149 | 1.00 | 49.18 | 8 |
| ATOM | 348 | N | LYS | A | 44 | 48.324 | 47.118 | 63.992 | 1.00 | 49.40 | 7 |
| ATOM | 349 | CA | LYS | A | 44 | 48.730 | 45.949 | 64.762 | 1.00 | 49.09 | 6 |
| ATOM | 350 | CB | LYS | A | 44 | 49.317 | 46.418 | 66.093 | 1.00 | 52.46 | 6 |
| ATOM | 351 | CG | LYS | A | 44 | 50.448 | 47.421 | 65.899 | 1.00 | 55.75 | 6 |
| ATOM | 352 | CD | LYS | A | 44 | 51.167 | 47.749 | 67.201 | 1.00 | 58.74 | 6 |
| ATOM | 353 | CE | LYS | A | 44 | 52.327 | 48.704 | 66.949 | 1.00 | 58.48 | 6 |
| ATOM | 354 | NZ | LYS | A | 44 | 53.122 | 48.968 | 68.176 | 1.00 | 58.95 | 7 |
| ATOM | 355 | C | LYS | A | 44 | 47.638 | 44.897 | 64.994 | 1.00 | 47.63 | 6 |
| ATOM | 356 | O | LYS | A | 44 | 47.932 | 43.738 | 65.290 | 1.00 | 45.13 | 8 |
| ATOM | 357 | N | GLU | A | 45 | 46.379 | 45.298 | 64.854 | 1.00 | 45.25 | 7 |
| ATOM | 358 | CA | GLU | A | 45 | 45.268 | 44.374 | 65.046 | 1.00 | 43.09 | 6 |
| ATOM | 359 | CB | GLU | A | 45 | 44.024 | 45.143 | 65.514 | 1.00 | 41.19 | 6 |
| ATOM | 360 | CG | GLU | A | 45 | 44.192 | 45.859 | 66.844 | 1.00 | 36.83 | 6 |
| ATOM | 361 | CD | GLU | A | 45 | 43.003 | 46.741 | 67.204 | 1.00 | 38.92 | 6 |
| ATOM | 362 | OE1 | GLU | A | 45 | 42.707 | 47.701 | 66.447 | 1.00 | 37.30 | 8 |
| ATOM | 363 | OE2 | GLU | A | 45 | 42.368 | 46.479 | 68.253 | 1.00 | 36.33 | 8 |
| ATOM | 364 | C | GLU | A | 45 | 44.969 | 43.660 | 63.726 | 1.00 | 43.04 | 6 |
| ATOM | 365 | O | GLU | A | 45 | 44.480 | 42.523 | 63.699 | 1.00 | 45.03 | 8 |
| ATOM | 366 | N | LEU | A | 46 | 45.282 | 44.341 | 62.632 | 1.00 | 40.29 | 7 |
| ATOM | 367 | CA | LEU | A | 46 | 45.042 | 43.823 | 61.299 | 1.00 | 37.16 | 6 |
| ATOM | 368 | CB | LEU | A | 46 | 44.910 | 44.990 | 60.331 | 1.00 | 37.86 | 6 |
| ATOM | 369 | CG | LEU | A | 46 | 44.822 | 44.658 | 58.845 | 1.00 | 39.22 | 6 |
| ATOM | 370 | CD1 | LEU | A | 46 | 43.655 | 43.726 | 58.563 | 1.00 | 40.68 | 6 |
| ATOM | 371 | CD2 | LEU | A | 46 | 44.673 | 45.964 | 58.080 | 1.00 | 41.62 | 6 |
| ATOM | 372 | C | LEU | A | 46 | 46.090 | 42.860 | 60.774 | 1.00 | 36.54 | 6 |
| ATOM | 373 | O | LEU | A | 46 | 47.275 | 43.192 | 60.698 | 1.00 | 39.86 | 8 |
| ATOM | 374 | N | ILE | A | 47 | 45.646 | 41.662 | 60.406 | 1.00 | 33.49 | 7 |
| ATOM | 375 | CA | ILE | A | 47 | 46.540 | 40.657 | 59.844 | 1.00 | 30.51 | 6 |
| ATOM | 376 | CB | ILE | A | 47 | 46.333 | 39.253 | 60.491 | 1.00 | 34.31 | 6 |
| ATOM | 377 | CG2 | ILE | A | 47 | 47.346 | 38.262 | 59.930 | 1.00 | 32.16 | 6 |
| ATOM | 378 | CG1 | ILE | A | 47 | 46.504 | 39.328 | 62.010 | 1.00 | 32.65 | 6 |
| ATOM | 379 | CD1 | ILE | A | 47 | 47.858 | 39.846 | 62.448 | 1.00 | 38.97 | 6 |
| ATOM | 380 | C | ILE | A | 47 | 46.196 | 40.570 | 58.362 | 1.00 | 28.36 | 6 |
| ATOM | 381 | O | ILE | A | 47 | 45.037 | 40.342 | 58.003 | 1.00 | 26.11 | 8 |
| ATOM | 382 | N | LYS | A | 48 | 47.194 | 40.772 | 57.504 | 1.00 | 27.77 | 7 |
| ATOM | 383 | CA | LYS | A | 48 | 46.985 | 40.713 | 56.056 | 1.00 | 25.80 | 6 |
| ATOM | 384 | CB | LYS | A | 48 | 48.258 | 41.087 | 55.308 | 1.00 | 23.91 | 6 |
| ATOM | 385 | CG | LYS | A | 48 | 48.056 | 41.273 | 53.811 | 1.00 | 24.90 | 6 |
| ATOM | 386 | CD | LYS | A | 48 | 49.389 | 41.352 | 53.091 | 1.00 | 26.39 | 6 |
| ATOM | 387 | CE | LYS | A | 48 | 49.233 | 41.864 | 51.679 | 1.00 | 27.71 | 6 |
| ATOM | 388 | NZ | LYS | A | 48 | 48.774 | 43.275 | 51.696 | 1.00 | 32.59 | 7 |
| ATOM | 389 | C | LYS | A | 48 | 46.595 | 39.299 | 55.654 | 1.00 | 26.32 | 6 |
| ATOM | 390 | O | LYS | A | 48 | 47.072 | 38.325 | 56.235 | 1.00 | 27.85 | 8 |
| ATOM | 391 | N | SER | A | 49 | 45.735 | 39.183 | 54.653 | 1.00 | 24.73 | 7 |
| ATOM | 392 | CA | SER | A | 49 | 45.299 | 37.876 | 54.205 | 1.00 | 27.36 | 6 |
| ATOM | 393 | CB | SER | A | 49 | 43.952 | 37.979 | 53.479 | 1.00 | 25.04 | 6 |
| ATOM | 394 | OG | SER | A | 49 | 42.911 | 38.329 | 54.373 | 1.00 | 26.94 | 8 |
| ATOM | 395 | C | SER | A | 49 | 46.322 | 37.211 | 53.293 | 1.00 | 28.97 | 6 |
| ATOM | 396 | O | SER | A | 49 | 47.095 | 37.885 | 52.612 | 1.00 | 31.89 | 8 |

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Figure 17-7

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 397 | N | ARG | A | 50 | 46.315 | 35.879 | 53.296 | 1.00 | 29.71 | 7 |
| ATOM | 398 | CA | ARG | A | 50 | 47.211 | 35.087 | 52.463 | 1.00 | 25.78 | 6 |
| ATOM | 399 | CB | ARG | A | 50 | 48.249 | 34.351 | 53.318 | 1.00 | 26.20 | 6 |
| ATOM | 400 | CG | ARG | A | 50 | 47.687 | 33.204 | 54.172 | 1.00 | 22.71 | 6 |
| ATOM | 401 | CD | ARG | A | 50 | 48.818 | 32.468 | 54.890 | 1.00 | 22.95 | 6 |
| ATOM | 402 | NE | ARG | A | 50 | 48.359 | 31.385 | 55.762 | 1.00 | 19.20 | 7 |
| ATOM | 403 | CZ | ARG | A | 50 | 47.708 | 30.306 | 55.345 | 1.00 | 16.85 | 6 |
| ATOM | 404 | NH1 | ARG | A | 50 | 47.430 | 30.151 | 54.055 | 1.00 | 17.77 | 7 |
| ATOM | 405 | NH2 | ARG | A | 50 | 47.334 | 29.385 | 56.223 | 1.00 | 14.56 | 7 |
| ATOM | 406 | C | ARG | A | 50 | 46.370 | 34.051 | 51.723 | 1.00 | 23.30 | 6 |
| ATOM | 407 | O | ARG | A | 50 | 45.319 | 33.635 | 52.206 | 1.00 | 16.92 | 8 |
| ATOM | 408 | N | PRO | A | 51 | 46.823 | 33.628 | 50.534 | 1.00 | 21.06 | 7 |
| ATOM | 409 | CD | PRO | A | 51 | 48.021 | 34.038 | 49.789 | 1.00 | 20.50 | 6 |
| ATOM | 410 | CA | PRO | A | 51 | 46.086 | 32.633 | 49.761 | 1.00 | 22.69 | 6 |
| ATOM | 411 | CB | PRO | A | 51 | 46.862 | 32.592 | 48.451 | 1.00 | 21.57 | 6 |
| ATOM | 412 | CG | PRO | A | 51 | 47.503 | 33.984 | 48.392 | 1.00 | 20.57 | 6 |
| ATOM | 413 | C | PRO | A | 51 | 46.153 | 31.300 | 50.498 | 1.00 | 26.71 | 6 |
| ATOM | 414 | O | PRO | A | 51 | 47.071 | 31.066 | 51.293 | 1.00 | 31.32 | 8 |
| ATOM | 415 | N | ALA | A | 52 | 45.176 | 30.435 | 50.250 | 1.00 | 26.02 | 7 |
| ATOM | 416 | CA | ALA | A | 52 | 45.151 | 29.121 | 50.876 | 1.00 | 25.76 | 6 |
| ATOM | 417 | CB | ALA | A | 52 | 43.720 | 28.585 | 50.933 | 1.00 | 21.42 | 6 |
| ATOM | 418 | C | ALA | A | 52 | 46.013 | 28.227 | 50.000 | 1.00 | 26.31 | 6 |
| ATOM | 419 | O | ALA | A | 52 | 45.878 | 28.239 | 48.780 | 1.00 | 30.31 | 8 |
| ATOM | 420 | N | THR | A | 53 | 46.909 | 27.464 | 50.608 | 1.00 | 26.80 | 7 |
| ATOM | 421 | CA | THR | A | 53 | 47.759 | 26.578 | 49.831 | 1.00 | 27.52 | 6 |
| ATOM | 422 | CB | THR | A | 53 | 48.845 | 25.975 | 50.717 | 1.00 | 26.27 | 6 |
| ATOM | 423 | OG1 | THR | A | 53 | 48.255 | 25.053 | 51.641 | 1.00 | 29.51 | 8 |
| ATOM | 424 | CG2 | THR | A | 53 | 49.522 | 27.076 | 51.502 | 1.00 | 24.66 | 6 |
| ATOM | 425 | C | THR | A | 53 | 46.908 | 25.462 | 49.209 | 1.00 | 26.58 | 6 |
| ATOM | 426 | O | THR | A | 53 | 45.778 | 25.228 | 49.634 | 1.00 | 21.98 | 8 |
| ATOM | 427 | N | LYS | A | 54 | 47.455 | 24.782 | 48.203 | 1.00 | 29.62 | 7 |
| ATOM | 428 | CA | LYS | A | 54 | 46.739 | 23.713 | 47.507 | 1.00 | 32.62 | 6 |
| ATOM | 429 | CB | LYS | A | 54 | 47.601 | 23.151 | 46.370 | 1.00 | 31.99 | 6 |
| ATOM | 430 | CG | LYS | A | 54 | 46.985 | 21.967 | 45.629 | 1.00 | 36.62 | 6 |
| ATOM | 431 | CD | LYS | A | 54 | 45.733 | 22.352 | 44.866 | 1.00 | 40.69 | 6 |
| ATOM | 432 | CE | LYS | A | 54 | 46.058 | 23.173 | 43.625 | 1.00 | 46.44 | 6 |
| ATOM | 433 | NZ | LYS | A | 54 | 46.844 | 22.393 | 42.614 | 1.00 | 50.68 | 7 |
| ATOM | 434 | C | LYS | A | 54 | 46.348 | 22.595 | 48.465 | 1.00 | 36.00 | 6 |
| ATOM | 435 | O | LYS | A | 54 | 45.277 | 21.991 | 48.330 | 1.00 | 34.77 | 8 |
| ATOM | 436 | N | GLU | A | 55 | 47.216 | 22.336 | 49.443 | 1.00 | 37.91 | 7 |
| ATOM | 437 | CA | GLU | A | 55 | 46.979 | 21.290 | 50.433 | 1.00 | 36.96 | 6 |
| ATOM | 438 | CB | GLU | A | 55 | 48.240 | 21.100 | 51.281 | 1.00 | 40.29 | 6 |
| ATOM | 439 | CG | GLU | A | 55 | 48.216 | 19.687 | 52.195 | 1.00 | 47.95 | 6 |
| ATOM | 440 | CD | GLU | A | 55 | 49.552 | 19.654 | 52.891 | 1.00 | 51.01 | 6 |
| ATOM | 441 | OE1 | GLU | A | 55 | 49.659 | 18.688 | 53.679 | 1.00 | 52.65 | 8 |
| ATOM | 442 | OE2 | GLU | A | 55 | 50.497 | 20.437 | 52.646 | 1.00 | 51.27 | 8 |
| ATOM | 443 | C | GLU | A | 55 | 45.771 | 21.609 | 51.322 | 1.00 | 34.10 | 6 |
| ATOM | 444 | O | GLU | A | 55 | 44.892 | 20.769 | 51.496 | 1.00 | 33.08 | 8 |
| ATOM | 445 | N | GLU | A | 56 | 45.723 | 22.827 | 51.866 | 1.00 | 32.39 | 7 |
| ATOM | 446 | CA | GLU | A | 56 | 44.621 | 23.256 | 52.733 | 1.00 | 30.13 | 6 |
| ATOM | 447 | CB | GLU | A | 56 | 44.824 | 24.714 | 53.177 | 1.00 | 25.28 | 6 |
| ATOM | 448 | CG | GLU | A | 56 | 46.204 | 24.994 | 53.758 | 1.00 | 28.82 | 6 |
| ATOM | 449 | CD | GLU | A | 56 | 46.421 | 26.450 | 54.181 | 1.00 | 30.74 | 6 |
| ATOM | 450 | OE1 | GLU | A | 56 | 46.072 | 27.369 | 53.398 | 1.00 | 29.77 | 8 |
| ATOM | 451 | OE2 | GLU | A | 56 | 46.969 | 26.674 | 55.288 | 1.00 | 25.98 | 8 |
| ATOM | 452 | C | GLU | A | 56 | 43.264 | 23.114 | 52.024 | 1.00 | 29.63 | 6 |
| ATOM | 453 | O | GLU | A | 56 | 42.299 | 22.584 | 52.595 | 1.00 | 29.90 | 8 |
| ATOM | 454 | N | LEU | A | 57 | 43.188 | 23.581 | 50.780 | 1.00 | 26.76 | 7 |
| ATOM | 455 | CA | LEU | A | 57 | 41.944 | 23.490 | 50.020 | 1.00 | 25.29 | 6 |
| ATOM | 456 | CB | LEU | A | 57 | 42.132 | 24.103 | 48.629 | 1.00 | 22.68 | 6 |
| ATOM | 457 | CG | LEU | A | 57 | 42.402 | 25.612 | 48.572 | 1.00 | 22.39 | 6 |
| ATOM | 458 | CD1 | LEU | A | 57 | 42.654 | 26.045 | 47.123 | 1.00 | 20.77 | 6 |
| ATOM | 459 | CD2 | LEU | A | 57 | 41.211 | 26.366 | 49.156 | 1.00 | 17.66 | 6 |
| ATOM | 460 | C | LEU | A | 57 | 41.479 | 22.037 | 49.896 | 1.00 | 26.02 | 6 |
| ATOM | 461 | O | LEU | A | 57 | 40.284 | 21.741 | 50.014 | 1.00 | 23.41 | 8 |
| ATOM | 462 | N | LEU | A | 58 | 42.444 | 21.143 | 49.675 | 1.00 | 24.82 | 7 |

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Figure 17-8

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 463 | CA | LEU | A | 58 | 42.194 | 19.718 | 49.526 | 1.00 | 22.44 | 6 |
| ATOM | 464 | CB | LEU | A | 58 | 43.434 | 19.027 | 48.965 | 1.00 | 21.02 | 6 |
| ATOM | 465 | CG | LEU | A | 58 | 43.838 | 19.471 | 47.558 | 1.00 | 22.94 | 6 |
| ATOM | 466 | CD1 | LEU | A | 58 | 45.212 | 18.908 | 47.176 | 1.00 | 20.35 | 6 |
| ATOM | 467 | CD2 | LEU | A | 58 | 42.755 | 19.033 | 46.587 | 1.00 | 23.28 | 6 |
| ATOM | 468 | C | LEU | A | 58 | 41.797 | 19.054 | 50.835 | 1.00 | 25.20 | 6 |
| ATOM | 469 | O | LEU | A | 58 | 41.456 | 17.867 | 50.854 | 1.00 | 26.55 | 8 |
| ATOM | 470 | N | LEU | A | 59 | 41.858 | 19.794 | 51.938 | 1.00 | 25.44 | 7 |
| ATOM | 471 | CA | LEU | A | 59 | 41.446 | 19.212 | 53.211 | 1.00 | 25.24 | 6 |
| ATOM | 472 | CB | LEU | A | 59 | 41.559 | 20.229 | 54.350 | 1.00 | 24.68 | 6 |
| ATOM | 473 | CG | LEU | A | 59 | 42.956 | 20.490 | 54.912 | 1.00 | 27.05 | 6 |
| ATOM | 474 | CD1 | LEU | A | 59 | 42.912 | 21.565 | 56.001 | 1.00 | 24.76 | 6 |
| ATOM | 475 | CD2 | LEU | A | 59 | 43.492 | 19.184 | 55.474 | 1.00 | 26.99 | 6 |
| ATOM | 476 | C | LEU | A | 59 | 39.991 | 18.807 | 53.045 | 1.00 | 24.22 | 6 |
| ATOM | 477 | O | LEU | A | 59 | 39.548 | 17.794 | 53.581 | 1.00 | 21.18 | 8 |
| ATOM | 478 | N | PHE | A | 60 | 39.270 | 19.615 | 52.270 | 1.00 | 25.00 | 7 |
| ATOM | 479 | CA | PHE | A | 60 | 37.859 | 19.403 | 52.011 | 1.00 | 25.00 | 6 |
| ATOM | 480 | CB | PHE | A | 60 | 37.054 | 20.560 | 52.605 | 1.00 | 26.34 | 6 |
| ATOM | 481 | CG | PHE | A | 60 | 35.600 | 20.555 | 52.223 | 1.00 | 29.37 | 6 |
| ATOM | 482 | CD1 | PHE | A | 60 | 34.811 | 19.422 | 52.427 | 1.00 | 27.57 | 6 |
| ATOM | 483 | CD2 | PHE | A | 60 | 35.015 | 21.692 | 51.661 | 1.00 | 27.33 | 6 |
| ATOM | 484 | CE1 | PHE | A | 60 | 33.466 | 19.419 | 52.077 | 1.00 | 27.00 | 6 |
| ATOM | 485 | CE2 | PHE | A | 60 | 33.670 | 21.699 | 51.306 | 1.00 | 28.08 | 6 |
| ATOM | 486 | CZ | PHE | A | 60 | 32.893 | 20.559 | 51.513 | 1.00 | 29.48 | 6 |
| ATOM | 487 | C | PHE | A | 60 | 37.506 | 19.214 | 50.538 | 1.00 | 27.78 | 6 |
| ATOM | 488 | O | PHE | A | 60 | 37.022 | 18.143 | 50.158 | 1.00 | 31.57 | 8 |
| ATOM | 489 | N | HIS | A | 61 | 37.734 | 20.220 | 49.696 | 1.00 | 26.76 | 7 |
| ATOM | 490 | CA | HIS | A | 61 | 37.376 | 20.056 | 48.287 | 1.00 | 28.84 | 6 |
| ATOM | 491 | CB | HIS | A | 61 | 37.365 | 21.405 | 47.561 | 1.00 | 27.76 | 6 |
| ATOM | 492 | CG | HIS | A | 61 | 36.385 | 22.396 | 48.117 | 1.00 | 30.54 | 6 |
| ATOM | 493 | CD2 | HIS | A | 61 | 35.056 | 22.549 | 47.907 | 1.00 | 33.74 | 6 |
| ATOM | 494 | ND1 | HIS | A | 61 | 36.750 | 23.401 | 48.987 | 1.00 | 34.02 | 7 |
| ATOM | 495 | CE1 | HIS | A | 61 | 35.691 | 24.135 | 49.286 | 1.00 | 32.07 | 6 |
| ATOM | 496 | NE2 | HIS | A | 61 | 34.649 | 23.638 | 48.644 | 1.00 | 34.10 | 7 |
| ATOM | 497 | C | HIS | A | 61 | 38.278 | 19.056 | 47.539 | 1.00 | 28.38 | 6 |
| ATOM | 498 | O | HIS | A | 61 | 39.287 | 18.604 | 48.072 | 1.00 | 25.81 | 8 |
| ATOM | 499 | N | THR | A | 62 | 37.895 | 18.705 | 46.310 | 1.00 | 32.88 | 7 |
| ATOM | 500 | CA | THR | A | 62 | 38.658 | 17.749 | 45.488 | 1.00 | 34.68 | 6 |
| ATOM | 501 | CB | THR | A | 62 | 37.715 | 16.739 | 44.778 | 1.00 | 34.36 | 6 |
| ATOM | 502 | OG1 | THR | A | 62 | 36.942 | 17.415 | 43.778 | 1.00 | 34.81 | 8 |
| ATOM | 503 | CG2 | THR | A | 62 | 36.759 | 16.112 | 45.778 | 1.00 | 34.33 | 6 |
| ATOM | 504 | C | THR | A | 62 | 39.485 | 18.454 | 44.408 | 1.00 | 35.60 | 6 |
| ATOM | 505 | O | THR | A | 62 | 39.017 | 19.418 | 43.790 | 1.00 | 30.85 | 8 |
| ATOM | 506 | N | GLU | A | 63 | 40.700 | 17.958 | 44.166 | 1.00 | 37.38 | 7 |
| ATOM | 507 | CA | GLU | A | 63 | 41.587 | 18.555 | 43.165 | 1.00 | 40.68 | 6 |
| ATOM | 508 | CB | GLU | A | 63 | 42.759 | 17.626 | 42.840 | 1.00 | 43.75 | 6 |
| ATOM | 509 | CG | GLU | A | 63 | 43.719 | 17.389 | 43.987 | 1.00 | 50.68 | 6 |
| ATOM | 510 | CD | GLU | A | 63 | 45.026 | 16.760 | 43.529 | 1.00 | 55.36 | 6 |
| ATOM | 511 | OE1 | GLU | A | 63 | 45.789 | 17.441 | 42.808 | 1.00 | 53.03 | 8 |
| ATOM | 512 | OE2 | GLU | A | 63 | 45.285 | 15.585 | 43.883 | 1.00 | 59.56 | 8 |
| ATOM | 513 | C | GLU | A | 63 | 40.894 | 18.939 | 41.860 | 1.00 | 39.26 | 6 |
| ATOM | 514 | O | GLU | A | 63 | 40.771 | 20.116 | 41.535 | 1.00 | 42.33 | 8 |
| ATOM | 515 | N | ASP | A | 64 | 40.453 | 17.948 | 41.102 | 1.00 | 37.07 | 7 |
| ATOM | 516 | CA | ASP | A | 64 | 39.782 | 18.224 | 39.845 | 1.00 | 36.98 | 6 |
| ATOM | 517 | CB | ASP | A | 64 | 38.957 | 17.000 | 39.426 | 1.00 | 42.19 | 6 |
| ATOM | 518 | CG | ASP | A | 64 | 38.037 | 16.501 | 40.533 | 1.00 | 47.66 | 6 |
| ATOM | 519 | OD1 | ASP | A | 64 | 37.039 | 17.193 | 40.851 | 1.00 | 47.95 | 8 |
| ATOM | 520 | OD2 | ASP | A | 64 | 38.325 | 15.413 | 41.091 | 1.00 | 50.07 | 8 |
| ATOM | 521 | C | ASP | A | 64 | 38.908 | 19.480 | 39.906 | 1.00 | 33.40 | 6 |
| ATOM | 522 | O | ASP | A | 64 | 38.927 | 20.293 | 38.986 | 1.00 | 33.64 | 8 |
| ATOM | 523 | N | TYR | A | 65 | 38.156 | 19.641 | 40.990 | 1.00 | 30.57 | 7 |
| ATOM | 524 | CA | TYR | A | 65 | 37.286 | 20.806 | 41.157 | 1.00 | 29.65 | 6 |
| ATOM | 525 | CB | TYR | A | 65 | 36.300 | 20.560 | 42.316 | 1.00 | 30.16 | 6 |
| ATOM | 526 | CG | TYR | A | 65 | 35.557 | 21.790 | 42.810 | 1.00 | 28.49 | 6 |
| ATOM | 527 | CD1 | TYR | A | 65 | 34.791 | 22.572 | 41.944 | 1.00 | 30.25 | 6 |
| ATOM | 528 | CE1 | TYR | A | 65 | 34.126 | 23.715 | 42.399 | 1.00 | 28.36 | 6 |

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Figure 17-9

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 529 | CD2 | TYR | A | 65 | 35.638 | 22.181 | 44.150 | 1.00 | 28.28 | 6 |
| ATOM | 530 | CE2 | TYR | A | 65 | 34.980 | 23.320 | 44.617 | 1.00 | 26.96 | 6 |
| ATOM | 531 | CZ | TYR | A | 65 | 34.227 | 24.082 | 43.740 | 1.00 | 29.79 | 6 |
| ATOM | 532 | OH | TYR | A | 65 | 33.568 | 25.201 | 44.207 | 1.00 | 28.53 | 8 |
| ATOM | 533 | C | TYR | A | 65 | 38.118 | 22.061 | 41.418 | 1.00 | 29.15 | 6 |
| ATOM | 534 | O | TYR | A | 65 | 37.860 | 23.128 | 40.857 | 1.00 | 30.45 | 8 |
| ATOM | 535 | N | ILE | A | 66 | 39.122 | 21.926 | 42.270 | 1.00 | 26.61 | 7 |
| ATOM | 536 | CA | ILE | A | 66 | 39.986 | 23.041 | 42.597 | 1.00 | 26.35 | 6 |
| ATOM | 537 | CB | ILE | A | 66 | 40.998 | 22.652 | 43.687 | 1.00 | 26.25 | 6 |
| ATOM | 538 | CG2 | ILE | A | 66 | 42.009 | 23.753 | 43.869 | 1.00 | 21.20 | 6 |
| ATOM | 539 | CG1 | ILE | A | 66 | 40.264 | 22.341 | 44.992 | 1.00 | 29.30 | 6 |
| ATOM | 540 | CD1 | ILE | A | 66 | 39.478 | 23.517 | 45.555 | 1.00 | 30.52 | 6 |
| ATOM | 541 | C | ILE | A | 66 | 40.761 | 23.504 | 41.381 | 1.00 | 28.07 | 6 |
| ATOM | 542 | O | ILE | A | 66 | 41.039 | 24.696 | 41.225 | 1.00 | 31.26 | 8 |
| ATOM | 543 | N | ASN | A | 67 | 41.125 | 22.559 | 40.521 | 1.00 | 28.47 | 7 |
| ATOM | 544 | CA | ASN | A | 67 | 41.902 | 22.898 | 39.337 | 1.00 | 30.15 | 6 |
| ATOM | 545 | CB | ASN | A | 67 | 42.563 | 21.656 | 38.726 | 1.00 | 34.20 | 6 |
| ATOM | 546 | CG | ASN | A | 67 | 43.712 | 21.118 | 39.578 | 1.00 | 38.78 | 6 |
| ATOM | 547 | OD1 | ASN | A | 67 | 44.674 | 21.841 | 39.878 | 1.00 | 43.34 | 8 |
| ATOM | 548 | ND2 | ASN | A | 67 | 43.626 | 19.845 | 39.956 | 1.00 | 37.14 | 7 |
| ATOM | 549 | C | ASN | A | 67 | 41.020 | 23.554 | 38.314 | 1.00 | 28.41 | 6 |
| ATOM | 550 | O | ASN | A | 67 | 41.494 | 24.354 | 37.499 | 1.00 | 28.05 | 8 |
| ATOM | 551 | N | THR | A | 68 | 39.733 | 23.221 | 38.361 | 1.00 | 25.32 | 7 |
| ATOM | 552 | CA | THR | A | 68 | 38.787 | 23.791 | 37.416 | 1.00 | 21.75 | 6 |
| ATOM | 553 | CB | THR | A | 68 | 37.438 | 23.111 | 37.500 | 1.00 | 16.99 | 6 |
| ATOM | 554 | OG1 | THR | A | 68 | 37.620 | 21.695 | 37.371 | 1.00 | 16.99 | 8 |
| ATOM | 555 | CG2 | THR | A | 68 | 36.549 | 23.591 | 36.359 | 1.00 | 17.59 | 6 |
| ATOM | 556 | C | THR | A | 68 | 38.633 | 25.263 | 37.732 | 1.00 | 22.13 | 6 |
| ATOM | 557 | O | THR | A | 68 | 38.529 | 26.088 | 36.830 | 1.00 | 21.97 | 8 |
| ATOM | 558 | N | LEU | A | 69 | 38.645 | 25.582 | 39.023 | 1.00 | 22.32 | 7 |
| ATOM | 559 | CA | LEU | A | 69 | 38.535 | 26.956 | 39.482 | 1.00 | 23.97 | 6 |
| ATOM | 560 | CB | LEU | A | 69 | 38.376 | 26.982 | 41.000 | 1.00 | 24.99 | 6 |
| ATOM | 561 | CG | LEU | A | 69 | 37.023 | 26.527 | 41.548 | 1.00 | 29.08 | 6 |
| ATOM | 562 | CD1 | LEU | A | 69 | 37.087 | 26.416 | 43.066 | 1.00 | 30.99 | 6 |
| ATOM | 563 | CD2 | LEU | A | 69 | 35.942 | 27.528 | 41.120 | 1.00 | 28.69 | 6 |
| ATOM | 564 | C | LEU | A | 69 | 39.772 | 27.757 | 39.088 | 1.00 | 24.90 | 6 |
| ATOM | 565 | O | LEU | A | 69 | 39.683 | 28.921 | 38.674 | 1.00 | 25.04 | 8 |
| ATOM | 566 | N | MET | A | 70 | 40.932 | 27.128 | 39.218 | 1.00 | 24.67 | 7 |
| ATOM | 567 | CA | MET | A | 70 | 42.183 | 27.794 | 38.897 | 1.00 | 23.62 | 6 |
| ATOM | 568 | CB | MET | A | 70 | 43.358 | 26.953 | 39.380 | 1.00 | 26.92 | 6 |
| ATOM | 569 | CG | MET | A | 70 | 43.418 | 26.751 | 40.884 | 1.00 | 26.69 | 6 |
| ATOM | 570 | SD | MET | A | 70 | 44.970 | 25.929 | 41.325 | 1.00 | 30.71 | 16 |
| ATOM | 571 | CE | MET | A | 70 | 46.137 | 27.077 | 40.642 | 1.00 | 23.20 | 6 |
| ATOM | 572 | C | MET | A | 70 | 42.324 | 28.040 | 37.412 | 1.00 | 21.62 | 6 |
| ATOM | 573 | O | MET | A | 70 | 42.903 | 29.041 | 36.982 | 1.00 | 18.99 | 8 |
| ATOM | 574 | N | GLU | A | 71 | 41.769 | 27.122 | 36.632 | 1.00 | 23.93 | 7 |
| ATOM | 575 | CA | GLU | A | 71 | 41.859 | 27.204 | 36.189 | 1.00 | 24.41 | 6 |
| ATOM | 576 | CB | GLU | A | 71 | 41.681 | 25.814 | 34.582 | 1.00 | 26.22 | 6 |
| ATOM | 577 | CG | GLU | A | 71 | 42.224 | 25.695 | 33.167 | 1.00 | 31.75 | 6 |
| ATOM | 578 | CD | GLU | A | 71 | 43.737 | 25.905 | 33.099 | 1.00 | 33.00 | 6 |
| ATOM | 579 | OE1 | GLU | A | 71 | 44.288 | 25.855 | 31.983 | 1.00 | 35.84 | 8 |
| ATOM | 580 | OE2 | GLU | A | 71 | 44.377 | 26.116 | 34.154 | 1.00 | 30.13 | 8 |
| ATOM | 581 | C | GLU | A | 71 | 40.845 | 28.160 | 34.592 | 1.00 | 21.86 | 6 |
| ATOM | 582 | O | GLU | A | 71 | 41.144 | 28.851 | 33.626 | 1.00 | 21.54 | 8 |
| ATOM | 583 | N | ALA | A | 72 | 39.649 | 28.197 | 35.169 | 1.00 | 19.22 | 7 |
| ATOM | 584 | CA | ALA | A | 72 | 38.589 | 29.067 | 34.684 | 1.00 | 19.39 | 6 |
| ATOM | 585 | CB | ALA | A | 72 | 37.298 | 28.743 | 35.397 | 1.00 | 19.23 | 6 |
| ATOM | 586 | C | ALA | A | 72 | 38.931 | 30.536 | 34.899 | 1.00 | 26.72 | 6 |
| ATOM | 587 | O | ALA | A | 72 | 38.711 | 31.383 | 34.016 | 1.00 | 26.12 | 8 |
| ATOM | 588 | N | GLU | A | 73 | 39.470 | 30.835 | 36.079 | 1.00 | 28.44 | 7 |
| ATOM | 589 | CA | GLU | A | 73 | 39.820 | 32.202 | 36.436 | 1.00 | 29.44 | 6 |
| ATOM | 590 | CB | GLU | A | 73 | 40.157 | 32.282 | 37.931 | 1.00 | 25.84 | 6 |
| ATOM | 591 | CG | GLU | A | 73 | 40.646 | 33.655 | 38.349 | 1.00 | 27.51 | 6 |
| ATOM | 592 | CD | GLU | A | 73 | 40.840 | 33.806 | 39.841 | 1.00 | 29.38 | 6 |
| ATOM | 593 | OE1 | GLU | A | 73 | 39.841 | 33.776 | 40.582 | 1.00 | 32.49 | 8 |
| ATOM | 594 | OE2 | GLU | A | 73 | 41.996 | 33.960 | 40.277 | 1.00 | 31.77 | 8 |

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Figure 17-10

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 595 | C | GLU | A | 73 | 40.946 | 32.840 | 35.615 | 1.00 | 31.83 | 6 |
| ATOM | 596 | O | GLU | A | 73 | 40.859 | 34.024 | 35.259 | 1.00 | 33.52 | 8 |
| ATOM | 597 | N | ARG | A | 74 | 41.992 | 32.071 | 35.309 | 1.00 | 31.45 | 7 |
| ATOM | 598 | CA | ARG | A | 74 | 43.128 | 32.611 | 34.557 | 1.00 | 30.65 | 6 |
| ATOM | 599 | CB | ARG | A | 74 | 44.405 | 31.826 | 34.874 | 1.00 | 32.12 | 6 |
| ATOM | 600 | CG | ARG | A | 74 | 44.514 | 30.467 | 34.205 | 1.00 | 31.42 | 6 |
| ATOM | 601 | CD | ARG | A | 74 | 45.702 | 29.714 | 34.754 | 1.00 | 30.73 | 6 |
| ATOM | 602 | NE | ARG | A | 74 | 46.041 | 28.561 | 33.933 | 1.00 | 34.18 | 7 |
| ATOM | 603 | CZ | ARG | A | 74 | 46.646 | 28.634 | 32.748 | 1.00 | 35.55 | 6 |
| ATOM | 604 | NH1 | ARG | A | 74 | 46.989 | 29.818 | 32.232 | 1.00 | 29.64 | 7 |
| ATOM | 605 | NH2 | ARG | A | 74 | 46.906 | 27.514 | 32.079 | 1.00 | 34.07 | 7 |
| ATOM | 606 | C | ARG | A | 74 | 42.894 | 32.623 | 33.051 | 1.00 | 28.61 | 6 |
| ATOM | 607 | O | ARG | A | 74 | 43.431 | 33.465 | 32.338 | 1.00 | 24.38 | 8 |
| ATOM | 608 | N | CYS | A | 75 | 42.107 | 31.673 | 32.566 | 1.00 | 28.32 | 7 |
| ATOM | 609 | CA | CYS | A | 75 | 41.796 | 31.619 | 31.148 | 1.00 | 32.42 | 6 |
| ATOM | 610 | CB | CYS | A | 75 | 41.687 | 30.167 | 30.682 | 1.00 | 32.91 | 6 |
| ATOM | 611 | SG | CYS | A | 75 | 43.281 | 29.296 | 30.777 | 1.00 | 37.09 | 16 |
| ATOM | 612 | C | CYS | A | 75 | 40.489 | 32.382 | 30.956 | 1.00 | 33.10 | 6 |
| ATOM | 613 | O | CYS | A | 75 | 40.029 | 32.598 | 29.834 | 1.00 | 30.74 | 8 |
| ATOM | 614 | N | GLN | A | 76 | 39.914 | 32.787 | 32.088 | 1.00 | 34.42 | 7 |
| ATOM | 615 | CA | GLN | A | 76 | 38.691 | 33.575 | 32.144 | 1.00 | 33.20 | 6 |
| ATOM | 616 | CB | GLN | A | 76 | 38.986 | 34.962 | 31.578 | 1.00 | 32.09 | 6 |
| ATOM | 617 | CG | GLN | A | 76 | 38.089 | 36.064 | 32.094 | 1.00 | 39.46 | 6 |
| ATOM | 618 | CD | GLN | A | 76 | 38.479 | 36.541 | 33.480 | 1.00 | 41.47 | 6 |
| ATOM | 619 | OE1 | GLN | A | 76 | 38.574 | 35.755 | 34.426 | 1.00 | 45.02 | 8 |
| ATOM | 620 | NE2 | GLN | A | 76 | 38.703 | 37.846 | 33.606 | 1.00 | 42.22 | 7 |
| ATOM | 621 | C | GLN | A | 76 | 37.561 | 32.920 | 31.358 | 1.00 | 33.20 | 6 |
| ATOM | 622 | O | GLN | A | 76 | 36.732 | 33.598 | 30.760 | 1.00 | 34.19 | 8 |
| ATOM | 623 | N | CYS | A | 77 | 37.522 | 31.598 | 31.370 | 1.00 | 31.81 | 7 |
| ATOM | 624 | CA | CYS | A | 77 | 36.511 | 30.862 | 30.627 | 1.00 | 31.47 | 6 |
| ATOM | 625 | CB | CYS | A | 77 | 37.187 | 30.181 | 29.454 | 1.00 | 30.25 | 6 |
| ATOM | 626 | SG | CYS | A | 77 | 38.479 | 29.071 | 30.044 | 1.00 | 33.94 | 16 |
| ATOM | 627 | C | CYS | A | 77 | 35.851 | 29.795 | 31.498 | 1.00 | 31.97 | 6 |
| ATOM | 628 | O | CYS | A | 77 | 36.335 | 29.503 | 32.590 | 1.00 | 35.15 | 8 |
| ATOM | 629 | N | VAL | A | 78 | 34.750 | 29.216 | 31.018 | 1.00 | 30.78 | 7 |
| ATOM | 630 | CA | VAL | A | 78 | 34.069 | 28.139 | 31.747 | 1.00 | 30.55 | 6 |
| ATOM | 631 | CB | VAL | A | 78 | 32.539 | 28.287 | 31.720 | 1.00 | 30.06 | 6 |
| ATOM | 632 | CG1 | VAL | A | 78 | 31.881 | 27.030 | 32.293 | 1.00 | 28.23 | 6 |
| ATOM | 633 | CG2 | VAL | A | 78 | 32.129 | 29.503 | 32.526 | 1.00 | 30.67 | 6 |
| ATOM | 634 | C | VAL | A | 78 | 34.420 | 26.794 | 31.110 | 1.00 | 29.80 | 6 |
| ATOM | 635 | O | VAL | A | 78 | 33.851 | 26.422 | 30.077 | 1.00 | 29.65 | 8 |
| ATOM | 636 | N | PRO | A | 79 | 35.337 | 26.033 | 31.739 | 1.00 | 28.55 | 7 |
| ATOM | 637 | CD | PRO | A | 79 | 35.985 | 26.335 | 33.025 | 1.00 | 24.39 | 6 |
| ATOM | 638 | CA | PRO | A | 79 | 35.793 | 24.724 | 31.261 | 1.00 | 28.89 | 6 |
| ATOM | 639 | CB | PRO | A | 79 | 36.622 | 24.218 | 32.434 | 1.00 | 24.49 | 6 |
| ATOM | 640 | CG | PRO | A | 79 | 37.239 | 25.500 | 32.922 | 1.00 | 25.68 | 6 |
| ATOM | 641 | C | PRO | A | 79 | 34.668 | 23.776 | 30.881 | 1.00 | 30.13 | 6 |
| ATOM | 642 | O | PRO | A | 79 | 33.697 | 23.624 | 31.615 | 1.00 | 30.87 | 8 |
| ATOM | 643 | N | LYS | A | 80 | 34.796 | 23.136 | 29.727 | 1.00 | 33.44 | 7 |
| ATOM | 644 | CA | LYS | A | 80 | 33.758 | 22.216 | 29.303 | 1.00 | 38.52 | 6 |
| ATOM | 645 | CB | LYS | A | 80 | 34.202 | 21.421 | 28.076 | 1.00 | 45.18 | 6 |
| ATOM | 646 | CG | LYS | A | 80 | 35.450 | 20.589 | 28.278 | 1.00 | 55.18 | 6 |
| ATOM | 647 | CD | LYS | A | 80 | 35.788 | 19.827 | 27.000 | 1.00 | 60.80 | 6 |
| ATOM | 648 | CE | LYS | A | 80 | 37.035 | 18.976 | 27.168 | 1.00 | 64.25 | 6 |
| ATOM | 649 | NZ | LYS | A | 80 | 37.367 | 18.252 | 25.911 | 1.00 | 68.95 | 7 |
| ATOM | 650 | C | LYS | A | 80 | 33.411 | 21.267 | 30.443 | 1.00 | 36.56 | 6 |
| ATOM | 651 | O | LYS | A | 80 | 34.293 | 20.775 | 31.164 | 1.00 | 31.61 | 8 |
| ATOM | 652 | N | GLY | A | 81 | 32.112 | 21.035 | 30.602 | 1.00 | 32.57 | 7 |
| ATOM | 653 | CA | GLY | A | 81 | 31.634 | 20.155 | 31.648 | 1.00 | 29.81 | 6 |
| ATOM | 654 | C | GLY | A | 81 | 31.477 | 20.884 | 32.965 | 1.00 | 28.30 | 6 |
| ATOM | 655 | O | GLY | A | 81 | 30.544 | 20.612 | 33.723 | 1.00 | 25.49 | 8 |
| ATOM | 656 | N | ALA | A | 82 | 32.380 | 21.830 | 33.218 | 1.00 | 25.99 | 7 |
| ATOM | 657 | CA | ALA | A | 82 | 32.384 | 22.602 | 34.458 | 1.00 | 26.72 | 6 |
| ATOM | 658 | CB | ALA | A | 82 | 33.485 | 23.674 | 34.406 | 1.00 | 22.64 | 6 |
| ATOM | 659 | C | ALA | A | 82 | 31.066 | 23.245 | 34.886 | 1.00 | 27.84 | 6 |
| ATOM | 660 | O | ALA | A | 82 | 30.729 | 23.224 | 36.068 | 1.00 | 30.00 | 8 |

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Figure 17-11

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 661 | N | ARG | A | 83 | 30.310 | 23.811 | 33.951 | 1.00 | 31.15 | 7 |
| ATOM | 662 | CA | ARG | A | 83 | 29.071 | 24.462 | 34.345 | 1.00 | 32.50 | 6 |
| ATOM | 663 | CB | ARG | A | 83 | 28.285 | 24.941 | 33.127 | 1.00 | 37.19 | 6 |
| ATOM | 664 | CG | ARG | A | 83 | 27.439 | 26.189 | 33.408 | 1.00 | 42.23 | 6 |
| ATOM | 665 | CD | ARG | A | 83 | 26.480 | 26.020 | 34.585 | 1.00 | 48.02 | 6 |
| ATOM | 666 | NE | ARG | A | 83 | 25.904 | 27.303 | 34.996 | 1.00 | 53.00 | 7 |
| ATOM | 667 | CZ | ARG | A | 83 | 25.046 | 27.460 | 36.005 | 1.00 | 56.84 | 6 |
| ATOM | 668 | NH1 | ARG | A | 83 | 24.649 | 26.413 | 36.724 | 1.00 | 53.05 | 7 |
| ATOM | 669 | NH2 | ARG | A | 83 | 24.588 | 28.672 | 36.304 | 1.00 | 58.03 | 7 |
| ATOM | 670 | C | ARG | A | 83 | 28.208 | 23.531 | 35.189 | 1.00 | 31.50 | 6 |
| ATOM | 671 | O | ARG | A | 83 | 28.056 | 23.749 | 36.386 | 1.00 | 29.62 | 8 |
| ATOM | 672 | N | GLU | A | 84 | 27.648 | 22.491 | 34.581 | 1.00 | 33.06 | 7 |
| ATOM | 673 | CA | GLU | A | 84 | 26.819 | 21.568 | 35.343 | 1.00 | 35.40 | 6 |
| ATOM | 674 | CB | GLU | A | 84 | 26.112 | 20.562 | 34.417 | 1.00 | 37.35 | 6 |
| ATOM | 675 | CG | GLU | A | 84 | 26.989 | 19.684 | 33.496 | 1.00 | 40.01 | 6 |
| ATOM | 676 | CD | GLU | A | 84 | 27.551 | 20.418 | 32.267 | 1.00 | 44.49 | 6 |
| ATOM | 677 | OE1 | GLU | A | 84 | 27.925 | 19.723 | 31.292 | 1.00 | 41.12 | 8 |
| ATOM | 678 | OE2 | GLU | A | 84 | 27.636 | 21.671 | 32.270 | 1.00 | 41.01 | 8 |
| ATOM | 679 | C | GLU | A | 84 | 27.617 | 20.823 | 36.417 | 1.00 | 35.42 | 6 |
| ATOM | 680 | O | GLU | A | 84 | 27.246 | 20.816 | 37.594 | 1.00 | 34.66 | 8 |
| ATOM | 681 | N | LYS | A | 85 | 28.727 | 20.226 | 36.002 | 1.00 | 35.21 | 7 |
| ATOM | 682 | CA | LYS | A | 85 | 29.604 | 19.450 | 36.878 | 1.00 | 37.93 | 6 |
| ATOM | 683 | CB | LYS | A | 85 | 30.841 | 19.030 | 36.076 | 1.00 | 40.61 | 6 |
| ATOM | 684 | CG | LYS | A | 85 | 31.739 | 17.977 | 36.706 | 1.00 | 42.63 | 6 |
| ATOM | 685 | CD | LYS | A | 85 | 31.038 | 16.640 | 36.872 | 1.00 | 45.48 | 6 |
| ATOM | 686 | CE | LYS | A | 85 | 32.054 | 15.523 | 37.078 | 1.00 | 45.60 | 6 |
| ATOM | 687 | NZ | LYS | A | 85 | 33.032 | 15.833 | 38.154 | 1.00 | 46.16 | 7 |
| ATOM | 688 | C | LYS | A | 85 | 30.032 | 20.159 | 38.175 | 1.00 | 37.56 | 6 |
| ATOM | 689 | O | LYS | A | 85 | 30.161 | 19.516 | 39.222 | 1.00 | 38.40 | 8 |
| ATOM | 690 | N | TYR | A | 86 | 30.254 | 21.472 | 38.116 | 1.00 | 35.60 | 7 |
| ATOM | 691 | CA | TYR | A | 86 | 30.671 | 22.216 | 39.307 | 1.00 | 32.67 | 6 |
| ATOM | 692 | CB | TYR | A | 86 | 32.151 | 22.610 | 39.200 | 1.00 | 32.09 | 6 |
| ATOM | 693 | CG | TYR | A | 86 | 33.065 | 21.424 | 38.995 | 1.00 | 33.63 | 6 |
| ATOM | 694 | CD1 | TYR | A | 86 | 33.120 | 20.393 | 39.932 | 1.00 | 32.12 | 6 |
| ATOM | 695 | CE1 | TYR | A | 86 | 33.918 | 19.266 | 39.723 | 1.00 | 33.59 | 6 |
| ATOM | 696 | CD2 | TYR | A | 86 | 33.839 | 21.306 | 37.841 | 1.00 | 33.82 | 6 |
| ATOM | 697 | CE2 | TYR | A | 86 | 34.645 | 20.178 | 37.623 | 1.00 | 34.55 | 6 |
| ATOM | 698 | CZ | TYR | A | 86 | 34.675 | 19.162 | 38.566 | 1.00 | 32.38 | 6 |
| ATOM | 699 | OH | TYR | A | 86 | 35.431 | 18.034 | 38.336 | 1.00 | 29.17 | 8 |
| ATOM | 700 | C | TYR | A | 86 | 29.831 | 23.455 | 39.597 | 1.00 | 30.21 | 6 |
| ATOM | 701 | O | TYR | A | 86 | 30.192 | 24.265 | 40.445 | 1.00 | 29.12 | 8 |
| ATOM | 702 | N | ASN | A | 87 | 28.712 | 23.594 | 38.893 | 1.00 | 29.44 | 7 |
| ATOM | 703 | CA | ASN | A | 87 | 27.797 | 24.717 | 39.086 | 1.00 | 28.58 | 6 |
| ATOM | 704 | CB | ASN | A | 87 | 27.154 | 24.618 | 40.470 | 1.00 | 25.63 | 6 |
| ATOM | 705 | CG | ASN | A | 87 | 25.871 | 25.428 | 40.596 | 1.00 | 28.05 | 6 |
| ATOM | 706 | OD1 | ASN | A | 87 | 25.275 | 25.477 | 41.672 | 1.00 | 21.32 | 8 |
| ATOM | 707 | ND2 | ASN | A | 87 | 25.434 | 26.055 | 39.506 | 1.00 | 18.35 | 7 |
| ATOM | 708 | C | ASN | A | 87 | 28.580 | 26.015 | 38.963 | 1.00 | 20.35 | 6 |
| ATOM | 709 | O | ASN | A | 87 | 28.319 | 26.981 | 39.677 | 1.00 | 32.07 | 8 |
| ATOM | 710 | N | ILE | A | 88 | 29.545 | 26.019 | 38.051 | 1.00 | 32.05 | 7 |
| ATOM | 711 | CA | ILE | A | 88 | 30.407 | 27.173 | 37.809 | 1.00 | 33.77 | 6 |
| ATOM | 712 | CB | ILE | A | 88 | 31.894 | 26.734 | 37.776 | 1.00 | 36.13 | 6 |
| ATOM | 713 | CG2 | ILE | A | 88 | 32.759 | 27.831 | 37.201 | 1.00 | 37.80 | 6 |
| ATOM | 714 | CG1 | ILE | A | 88 | 32.357 | 26.342 | 39.178 | 1.00 | 38.92 | 6 |
| ATOM | 715 | CD1 | ILE | A | 88 | 32.350 | 27.483 | 40.176 | 1.00 | 41.44 | 6 |
| ATOM | 716 | C | ILE | A | 88 | 30.085 | 27.857 | 36.482 | 1.00 | 32.28 | 6 |
| ATOM | 717 | O | ILE | A | 88 | 29.708 | 27.196 | 35.520 | 1.00 | 32.72 | 8 |
| ATOM | 718 | N | GLY | A | 89 | 30.237 | 29.179 | 36.438 | 1.00 | 31.56 | 7 |
| ATOM | 719 | CA | GLY | A | 89 | 29.994 | 29.915 | 35.207 | 1.00 | 30.84 | 6 |
| ATOM | 720 | C | GLY | A | 89 | 28.696 | 30.689 | 35.093 | 1.00 | 32.17 | 6 |
| ATOM | 721 | O | GLY | A | 89 | 28.628 | 31.670 | 34.349 | 1.00 | 30.42 | 8 |
| ATOM | 722 | N | GLY | A | 90 | 27.670 | 30.257 | 35.821 | 1.00 | 31.51 | 7 |
| ATOM | 723 | CA | GLY | A | 90 | 26.387 | 30.937 | 35.756 | 1.00 | 32.92 | 6 |
| ATOM | 724 | C | GLY | A | 90 | 26.316 | 32.246 | 36.524 | 1.00 | 34.32 | 6 |
| ATOM | 725 | O | GLY | A | 90 | 27.302 | 32.671 | 37.129 | 1.00 | 33.97 | 8 |
| ATOM | 726 | N | TYR | A | 91 | 25.144 | 32.862 | 36.504 | 1.00 | 33.88 | 7 |

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Figure 17-12

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 727 | CA | TYR | A | 91 | 24.924 | 34.146 | 37.206 | 1.00 | 35.76 | 6 |
| ATOM | 728 | CB | TYR | A | 91 | 23.465 | 34.589 | 37.058 | 1.00 | 38.10 | 6 |
| ATOM | 729 | CG | TYR | A | 91 | 23.089 | 35.733 | 37.990 | 1.00 | 42.40 | 6 |
| ATOM | 730 | CD1 | TYR | A | 91 | 23.417 | 37.057 | 37.688 | 1.00 | 43.57 | 6 |
| ATOM | 731 | CE1 | TYR | A | 91 | 23.105 | 38.106 | 38.577 | 1.00 | 42.44 | 6 |
| ATOM | 732 | CD2 | TYR | A | 91 | 22.444 | 35.484 | 39.205 | 1.00 | 44.07 | 6 |
| ATOM | 733 | CE2 | TYR | A | 91 | 22.132 | 36.526 | 40.097 | 1.00 | 42.67 | 6 |
| ATOM | 734 | CZ | TYR | A | 91 | 22.462 | 37.825 | 39.775 | 1.00 | 42.41 | 6 |
| ATOM | 735 | OH | TYR | A | 91 | 22.130 | 38.835 | 40.646 | 1.00 | 43.69 | 8 |
| ATOM | 736 | C | TYR | A | 91 | 25.242 | 34.082 | 38.701 | 1.00 | 34.15 | 6 |
| ATOM | 737 | O | TYR | A | 91 | 25.821 | 35.014 | 39.266 | 1.00 | 29.52 | 8 |
| ATOM | 738 | N | GLU | A | 92 | 24.837 | 32.986 | 39.333 | 1.00 | 34.78 | 7 |
| ATOM | 739 | CA | GLU | A | 92 | 25.024 | 32.797 | 40.767 | 1.00 | 38.46 | 6 |
| ATOM | 740 | CB | GLU | A | 92 | 24.233 | 31.564 | 41.211 | 1.00 | 43.99 | 6 |
| ATOM | 741 | CG | GLU | A | 92 | 23.932 | 31.489 | 42.700 | 1.00 | 52.10 | 6 |
| ATOM | 742 | CD | GLU | A | 92 | 23.294 | 30.161 | 43.097 | 1.00 | 58.00 | 6 |
| ATOM | 743 | OE1 | GLU | A | 92 | 24.001 | 29.126 | 43.058 | 1.00 | 60.63 | 8 |
| ATOM | 744 | OE2 | GLU | A | 92 | 22.087 | 30.149 | 43.434 | 1.00 | 59.58 | 8 |
| ATOM | 745 | C | GLU | A | 92 | 26.492 | 32.669 | 41.208 | 1.00 | 36.42 | 5 |
| ATOM | 746 | O | GLU | A | 92 | 26.902 | 33.287 | 42.193 | 1.00 | 32.92 | 8 |
| ATOM | 747 | N | ASN | A | 93 | 27.280 | 31.883 | 40.473 | 1.00 | 34.12 | 7 |
| ATOM | 748 | CA | ASN | A | 93 | 28.693 | 31.671 | 40.808 | 1.00 | 33.24 | 6 |
| ATOM | 749 | CB | ASN | A | 93 | 28.871 | 30.259 | 41.364 | 1.00 | 28.52 | 6 |
| ATOM | 750 | CG | ASN | A | 93 | 27.734 | 29.859 | 42.299 | 1.00 | 27.45 | 6 |
| ATOM | 751 | OD1 | ASN | A | 93 | 27.547 | 30.457 | 43.355 | 1.00 | 21.76 | 8 |
| ATOM | 752 | ND2 | ASN | A | 93 | 26.956 | 28.853 | 41.895 | 1.00 | 21.79 | 7 |
| ATOM | 753 | C | ASN | A | 93 | 29.529 | 31.843 | 39.535 | 1.00 | 35.04 | 6 |
| ATOM | 754 | O | ASN | A | 93 | 30.160 | 30.898 | 39.059 | 1.00 | 33.81 | 8 |
| ATOM | 755 | N | PRO | A | 94 | 29.583 | 33.081 | 39.010 | 1.00 | 36.19 | 7 |
| ATOM | 756 | CD | PRO | A | 94 | 28.970 | 34.231 | 39.690 | 1.00 | 34.62 | 6 |
| ATOM | 757 | CA | PRO | A | 94 | 30.274 | 33.560 | 37.808 | 1.00 | 34.80 | 6 |
| ATOM | 758 | CB | PRO | A | 94 | 29.924 | 35.050 | 37.791 | 1.00 | 33.94 | 6 |
| ATOM | 759 | CG | PRO | A | 94 | 28.619 | 35.095 | 38.516 | 1.00 | 36.13 | 6 |
| ATOM | 760 | C | PRO | A | 94 | 31.775 | 33.379 | 37.733 | 1.00 | 34.63 | 6 |
| ATOM | 761 | O | PRO | A | 94 | 32.443 | 33.103 | 38.730 | 1.00 | 34.72 | 8 |
| ATOM | 762 | N | VAL | A | 95 | 32.299 | 33.556 | 36.526 | 1.00 | 33.57 | 7 |
| ATOM | 763 | CA | VAL | A | 95 | 33.735 | 33.499 | 36.307 | 1.00 | 30.31 | 6 |
| ATOM | 764 | CB | VAL | A | 95 | 34.085 | 33.171 | 34.841 | 1.00 | 29.88 | 6 |
| ATOM | 765 | CG1 | VAL | A | 95 | 35.561 | 33.453 | 34.574 | 1.00 | 29.53 | 6 |
| ATOM | 766 | CG2 | VAL | A | 95 | 33.795 | 31.713 | 34.563 | 1.00 | 28.05 | 6 |
| ATOM | 767 | C | VAL | A | 95 | 34.195 | 34.910 | 36.624 | 1.00 | 29.86 | 6 |
| ATOM | 768 | O | VAL | A | 95 | 33.524 | 35.879 | 36.272 | 1.00 | 29.07 | 8 |
| ATOM | 769 | N | SER | A | 96 | 35.318 | 35.019 | 37.317 | 1.00 | 30.89 | 7 |
| ATOM | 770 | CA | SER | A | 96 | 35.889 | 36.310 | 37.687 | 1.00 | 32.27 | 6 |
| ATOM | 771 | CB | SER | A | 96 | 34.885 | 37.145 | 38.501 | 1.00 | 30.16 | 6 |
| ATOM | 772 | OG | SER | A | 96 | 34.600 | 36.545 | 39.756 | 1.00 | 26.77 | 8 |
| ATOM | 773 | C | SER | A | 96 | 37.111 | 35.993 | 38.537 | 1.00 | 32.96 | 6 |
| ATOM | 774 | O | SER | A | 96 | 37.603 | 34.865 | 38.511 | 1.00 | 33.77 | 8 |
| ATOM | 775 | N | TYR | A | 97 | 37.609 | 36.973 | 39.282 | 1.00 | 32.66 | 7 |
| ATOM | 776 | CA | TYR | A | 97 | 38.753 | 36.712 | 40.132 | 1.00 | 31.95 | 6 |
| ATOM | 777 | CB | TYR | A | 97 | 39.838 | 37.766 | 39.923 | 1.00 | 31.81 | 6 |
| ATOM | 778 | CG | TYR | A | 97 | 40.416 | 37.729 | 38.525 | 1.00 | 30.39 | 6 |
| ATOM | 779 | CD1 | TYR | A | 97 | 39.820 | 38.434 | 37.479 | 1.00 | 30.63 | 6 |
| ATOM | 780 | CE1 | TYR | A | 97 | 40.327 | 38.358 | 36.178 | 1.00 | 28.49 | 6 |
| ATOM | 781 | CD2 | TYR | A | 97 | 41.536 | 36.945 | 38.236 | 1.00 | 28.43 | 6 |
| ATOM | 782 | CE2 | TYR | A | 97 | 42.046 | 36.858 | 36.942 | 1.00 | 24.73 | 6 |
| ATOM | 783 | CZ | TYR | A | 97 | 41.437 | 37.565 | 35.919 | 1.00 | 27.27 | 6 |
| ATOM | 784 | OH | TYR | A | 97 | 41.915 | 37.455 | 34.633 | 1.00 | 26.70 | 8 |
| ATOM | 785 | C | TYR | A | 97 | 38.350 | 36.618 | 41.596 | 1.00 | 31.10 | 6 |
| ATOM | 786 | O | TYR | A | 97 | 39.178 | 36.735 | 42.495 | 1.00 | 33.01 | 8 |
| ATOM | 787 | N | ALA | A | 98 | 37.059 | 36.398 | 41.818 | 1.00 | 31.11 | 7 |
| ATOM | 788 | CA | ALA | A | 98 | 36.510 | 36.241 | 43.160 | 1.00 | 30.06 | 5 |
| ATOM | 789 | CB | ALA | A | 98 | 35.141 | 36.920 | 43.256 | 1.00 | 27.71 | 6 |
| ATOM | 790 | C | ALA | A | 98 | 36.350 | 34.736 | 43.357 | 1.00 | 31.24 | 6 |
| ATOM | 791 | O | ALA | A | 98 | 36.335 | 34.238 | 44.487 | 1.00 | 29.66 | 8 |
| ATOM | 792 | N | MET | A | 99 | 36.249 | 34.030 | 42.230 | 1.00 | 29.50 | 7 |

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Figure 17-13

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| ATOM | 793 | CA | MET | A | 99 | 36.048 | 32.589 | 42.207 | 1.00 | 29.89 | 6 |
| ATOM | 794 | CB | MET | A | 99 | 35.774 | 32.123 | 40.778 | 1.00 | 30.48 | 6 |
| ATOM | 795 | CG | MET | A | 99 | 36.942 | 32.265 | 39.822 | 1.00 | 29.63 | 6 |
| ATOM | 796 | SD | MET | A | 99 | 36.426 | 31.939 | 38.126 | 1.00 | 29.78 | 16 |
| ATOM | 797 | CE | MET | A | 99 | 35.629 | 30.273 | 38.347 | 1.00 | 25.05 | 6 |
| ATOM | 798 | C | MET | A | 99 | 37.199 | 31.800 | 42.783 | 1.00 | 30.81 | 6 |
| ATOM | 799 | O | MET | A | 99 | 36.993 | 30.757 | 43.406 | 1.00 | 30.59 | 8 |
| ATOM | 800 | N | PHE | A | 100 | 38.417 | 32.274 | 42.569 | 1.00 | 32.09 | 7 |
| ATOM | 801 | CA | PHE | A | 100 | 39.554 | 31.557 | 43.114 | 1.00 | 33.87 | 6 |
| ATOM | 802 | CB | PHE | A | 100 | 40.322 | 30.817 | 42.029 | 1.00 | 33.95 | 6 |
| ATOM | 803 | CG | PHE | A | 100 | 41.434 | 29.979 | 42.578 | 1.00 | 41.14 | 6 |
| ATOM | 804 | CD1 | PHE | A | 100 | 41.152 | 28.862 | 43.364 | 1.00 | 41.84 | 6 |
| ATOM | 805 | CD2 | PHE | A | 100 | 42.768 | 30.339 | 42.372 | 1.00 | 42.18 | 6 |
| ATOM | 806 | CE1 | PHE | A | 100 | 42.185 | 28.115 | 43.941 | 1.00 | 41.63 | 6 |
| ATOM | 807 | CE2 | PHE | A | 100 | 43.808 | 29.600 | 42.944 | 1.00 | 40.50 | 6 |
| ATOM | 808 | CZ | PHE | A | 100 | 43.517 | 28.487 | 43.729 | 1.00 | 39.89 | 6 |
| ATOM | 809 | C | PHE | A | 100 | 40.519 | 32.438 | 43.895 | 1.00 | 33.98 | 6 |
| ATOM | 810 | O | PHE | A | 100 | 40.706 | 32.231 | 45.088 | 1.00 | 38.21 | 8 |
| ATOM | 811 | N | THR | A | 101 | 41.137 | 33.415 | 43.245 | 1.00 | 28.09 | 7 |
| ATOM | 812 | CA | THR | A | 101 | 42.063 | 34.261 | 43.969 | 1.00 | 22.19 | 6 |
| ATOM | 813 | CB | THR | A | 101 | 42.623 | 35.378 | 43.072 | 1.00 | 22.48 | 6 |
| ATOM | 814 | OG1 | THR | A | 101 | 43.441 | 34.795 | 42.052 | 1.00 | 21.99 | 8 |
| ATOM | 815 | CG2 | THR | A | 101 | 43.468 | 36.335 | 43.876 | 1.00 | 15.00 | 6 |
| ATOM | 816 | C | THR | A | 101 | 41.408 | 34.860 | 45.205 | 1.00 | 21.71 | 6 |
| ATOM | 817 | O | THR | A | 101 | 41.988 | 34.845 | 46.282 | 1.00 | 23.82 | 8 |
| ATOM | 818 | N | GLY | A | 102 | 40.197 | 35.377 | 45.068 | 1.00 | 21.79 | 7 |
| ATOM | 819 | CA | GLY | A | 102 | 39.533 | 35.947 | 46.231 | 1.00 | 21.23 | 6 |
| ATOM | 820 | C | GLY | A | 102 | 39.072 | 34.833 | 47.153 | 1.00 | 23.03 | 6 |
| ATOM | 821 | O | GLY | A | 102 | 39.209 | 34.909 | 48.378 | 1.00 | 20.41 | 8 |
| ATOM | 822 | N | SER | A | 103 | 38.512 | 33.792 | 46.544 | 1.00 | 22.59 | 7 |
| ATOM | 823 | CA | SER | A | 103 | 38.028 | 32.640 | 47.276 | 1.00 | 26.51 | 6 |
| ATOM | 824 | CB | SER | A | 103 | 37.454 | 31.598 | 46.314 | 1.00 | 28.10 | 6 |
| ATOM | 825 | OG | SER | A | 103 | 36.314 | 32.099 | 45.639 | 1.00 | 32.01 | 8 |
| ATOM | 826 | C | SER | A | 103 | 39.188 | 32.040 | 48.032 | 1.00 | 27.73 | 6 |
| ATOM | 827 | O | SER | A | 103 | 39.019 | 31.544 | 49.144 | 1.00 | 30.61 | 8 |
| ATOM | 828 | N | SER | A | 104 | 40.364 | 32.080 | 47.410 | 1.00 | 28.76 | 7 |
| ATOM | 829 | CA | SER | A | 104 | 41.590 | 31.552 | 48.008 | 1.00 | 28.55 | 6 |
| ATOM | 830 | CB | SER | A | 104 | 42.769 | 31.683 | 47.039 | 1.00 | 28.74 | 6 |
| ATOM | 831 | OG | SER | A | 104 | 42.501 | 31.044 | 45.804 | 1.00 | 35.04 | 8 |
| ATOM | 832 | C | SER | A | 104 | 41.870 | 32.401 | 49.226 | 1.00 | 25.67 | 6 |
| ATOM | 833 | O | SER | A | 104 | 42.026 | 31.897 | 50.338 | 1.00 | 25.17 | 8 |
| ATOM | 834 | N | LEU | A | 105 | 41.909 | 33.705 | 48.986 | 1.00 | 23.91 | 7 |
| ATOM | 835 | CA | LEU | A | 105 | 42.163 | 34.698 | 50.008 | 1.00 | 23.01 | 6 |
| ATOM | 836 | CB | LEU | A | 105 | 42.049 | 36.082 | 49.382 | 1.00 | 23.57 | 6 |
| ATOM | 837 | CG | LEU | A | 105 | 43.158 | 37.091 | 49.672 | 1.00 | 26.30 | 6 |
| ATOM | 838 | CD1 | LEU | A | 105 | 44.502 | 36.551 | 49.178 | 1.00 | 22.38 | 6 |
| ATOM | 839 | CD2 | LEU | A | 105 | 42.823 | 38.413 | 48.984 | 1.00 | 27.36 | 6 |
| ATOM | 840 | C | LEU | A | 105 | 41.187 | 34.559 | 51.182 | 1.00 | 23.48 | 6 |
| ATOM | 841 | O | LEU | A | 105 | 41.604 | 34.448 | 52.331 | 1.00 | 21.60 | 8 |
| ATOM | 842 | N | ALA | A | 106 | 39.887 | 34.556 | 50.897 | 1.00 | 25.32 | 7 |
| ATOM | 843 | CA | ALA | A | 106 | 38.884 | 34.423 | 51.957 | 1.00 | 26.04 | 6 |
| ATOM | 844 | CB | ALA | A | 106 | 37.471 | 34.423 | 51.358 | 1.00 | 24.28 | 6 |
| ATOM | 845 | C | ALA | A | 106 | 39.088 | 33.158 | 52.790 | 1.00 | 25.76 | 6 |
| ATOM | 846 | O | ALA | A | 106 | 38.953 | 33.186 | 54.015 | 1.00 | 22.75 | 8 |
| ATOM | 847 | N | THR | A | 107 | 39.410 | 32.057 | 52.111 | 1.00 | 25.65 | 7 |
| ATOM | 848 | CA | THR | A | 107 | 39.620 | 30.760 | 52.754 | 1.00 | 25.54 | 6 |
| ATOM | 849 | CB | THR | A | 107 | 39.706 | 29.637 | 51.713 | 1.00 | 21.92 | 6 |
| ATOM | 850 | OG1 | THR | A | 107 | 38.559 | 29.688 | 50.868 | 1.00 | 26.40 | 8 |
| ATOM | 851 | CG2 | THR | A | 107 | 39.742 | 28.295 | 52.387 | 1.00 | 17.36 | 6 |
| ATOM | 852 | C | THR | A | 107 | 40.901 | 30.720 | 53.583 | 1.00 | 28.16 | 6 |
| ATOM | 853 | O | THR | A | 107 | 40.906 | 30.254 | 54.727 | 1.00 | 28.07 | 8 |
| ATOM | 854 | N | GLY | A | 108 | 41.994 | 31.191 | 52.996 | 1.00 | 28.51 | 7 |
| ATOM | 855 | CA | GLY | A | 108 | 43.247 | 31.187 | 53.718 | 1.00 | 28.37 | 6 |
| ATOM | 856 | C | GLY | A | 108 | 43.027 | 31.921 | 55.019 | 1.00 | 30.26 | 6 |
| ATOM | 857 | O | GLY | A | 108 | 43.502 | 31.499 | 56.076 | 1.00 | 32.98 | 8 |
| ATOM | 858 | N | SER | A | 109 | 42.283 | 33.018 | 54.942 | 1.00 | 24.81 | 7 |

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Figure 17-14

| | | | | | | | | | |
|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 859 | CA | SER A 109 | 42.002 | 33.810 | 56.119 | 1.00 | 24.86 | 6 |
| ATOM | 860 | CB | SER A 109 | 41.222 | 35.066 | 55.727 | 1.00 | 24.74 | 6 |
| ATOM | 861 | OG | SER A 109 | 41.992 | 35.898 | 54.872 | 1.00 | 21.07 | 8 |
| ATOM | 862 | C | SER A 109 | 41.240 | 32.996 | 57.173 | 1.00 | 27.89 | 6 |
| ATOM | 863 | O | SER A 109 | 41.424 | 33.214 | 58.377 | 1.00 | 30.92 | 8 |
| ATOM | 864 | N | THR A 110 | 40.389 | 32.064 | 56.744 | 1.00 | 23.91 | 7 |
| ATOM | 865 | CA | THR A 110 | 39.676 | 31.259 | 57.721 | 1.00 | 24.80 | 6 |
| ATOM | 866 | CB | THR A 110 | 38.641 | 30.290 | 57.074 | 1.00 | 29.65 | 6 |
| ATOM | 867 | OG1 | THR A 110 | 37.469 | 31.016 | 56.669 | 1.00 | 30.45 | 8 |
| ATOM | 868 | CG2 | THR A 110 | 38.228 | 29.205 | 58.067 | 1.00 | 29.00 | 6 |
| ATOM | 869 | C | THR A 110 | 40.712 | 30.449 | 58.478 | 1.00 | 24.34 | 6 |
| ATOM | 870 | O | THR A 110 | 40.615 | 30.282 | 59.699 | 1.00 | 24.74 | 8 |
| ATOM | 871 | N | VAL A 111 | 41.715 | 29.954 | 57.764 | 1.00 | 23.01 | 7 |
| ATOM | 872 | CA | VAL A 111 | 42.759 | 29.173 | 58.416 | 1.00 | 24.13 | 6 |
| ATOM | 873 | CB | VAL A 111 | 43.695 | 28.495 | 57.391 | 1.00 | 25.77 | 6 |
| ATOM | 874 | CG1 | VAL A 111 | 44.845 | 27.773 | 58.121 | 1.00 | 22.51 | 6 |
| ATOM | 875 | CG2 | VAL A 111 | 42.888 | 27.502 | 56.534 | 1.00 | 22.67 | 6 |
| ATOM | 876 | C | VAL A 111 | 43.576 | 30.071 | 59.329 | 1.00 | 23.14 | 6 |
| ATOM | 877 | O | VAL A 111 | 43.720 | 29.793 | 60.518 | 1.00 | 24.11 | 8 |
| ATOM | 878 | N | GLN A 112 | 44.101 | 31.156 | 58.772 | 1.00 | 24.94 | 7 |
| ATOM | 879 | CA | GLN A 112 | 44.895 | 32.100 | 59.554 | 1.00 | 25.12 | 6 |
| ATOM | 880 | CB | GLN A 112 | 45.082 | 33.413 | 58.779 | 1.00 | 25.14 | 6 |
| ATOM | 881 | CG | GLN A 112 | 45.545 | 33.224 | 57.330 | 1.00 | 28.51 | 6 |
| ATOM | 882 | CD | GLN A 112 | 45.789 | 34.534 | 56.594 | 1.00 | 29.13 | 6 |
| ATOM | 883 | OE1 | GLN A 112 | 46.779 | 35.219 | 56.837 | 1.00 | 31.22 | 8 |
| ATOM | 884 | NE2 | GLN A 112 | 44.877 | 34.890 | 55.694 | 1.00 | 29.31 | 7 |
| ATOM | 885 | C | GLN A 112 | 44.107 | 32.362 | 60.827 | 1.00 | 24.62 | 6 |
| ATOM | 886 | O | GLN A 112 | 44.647 | 32.311 | 61.939 | 1.00 | 21.10 | 8 |
| ATOM | 887 | N | ALA A 113 | 42.813 | 32.622 | 60.644 | 1.00 | 24.41 | 7 |
| ATOM | 888 | CA | ALA A 113 | 41.914 | 32.904 | 61.751 | 1.00 | 23.33 | 6 |
| ATOM | 889 | CB | ALA A 113 | 40.516 | 33.183 | 61.224 | 1.00 | 19.80 | 6 |
| ATOM | 890 | C | ALA A 113 | 41.901 | 31.733 | 62.729 | 1.00 | 25.34 | 6 |
| ATOM | 891 | O | ALA A 113 | 41.925 | 31.930 | 63.946 | 1.00 | 27.52 | 8 |
| ATOM | 892 | N | ILE A 114 | 41.859 | 30.509 | 62.211 | 1.00 | 24.39 | 7 |
| ATOM | 893 | CA | ILE A 114 | 41.867 | 29.356 | 63.106 | 1.00 | 24.49 | 6 |
| ATOM | 894 | CB | ILE A 114 | 41.524 | 28.042 | 62.371 | 1.00 | 23.46 | 6 |
| ATOM | 895 | CG2 | ILE A 114 | 41.902 | 26.855 | 63.227 | 1.00 | 18.97 | 6 |
| ATOM | 896 | CG1 | ILE A 114 | 40.030 | 28.015 | 62.034 | 1.00 | 21.17 | 6 |
| ATOM | 897 | CD1 | ILE A 114 | 39.598 | 26.791 | 61.239 | 1.00 | 22.51 | 6 |
| ATOM | 898 | C | ILE A 114 | 43.230 | 29.227 | 63.757 | 1.00 | 24.32 | 6 |
| ATOM | 899 | O | ILE A 114 | 43.328 | 28.817 | 64.907 | 1.00 | 24.74 | 8 |
| ATOM | 900 | N | GLU A 115 | 44.280 | 29.580 | 63.019 | 1.00 | 26.58 | 7 |
| ATOM | 901 | CA | GLU A 115 | 45.638 | 29.518 | 63.551 | 1.00 | 25.89 | 6 |
| ATOM | 902 | CB | GLU A 115 | 46.639 | 29.992 | 62.508 | 1.00 | 22.63 | 6 |
| ATOM | 903 | CG | GLU A 115 | 46.554 | 29.264 | 61.192 | 1.00 | 20.39 | 6 |
| ATOM | 904 | CD | GLU A 115 | 17.668 | 29.670 | 60.244 | 1.00 | 21.39 | 6 |
| ATOM | 905 | OE1 | GLU A 115 | 47.848 | 30.887 | 60.016 | 1.00 | 19.60 | 8 |
| ATOM | 906 | OE2 | GLU A 115 | 18.362 | 28.769 | 59.722 | 1.00 | 22.53 | 8 |
| ATOM | 907 | C | GLU A 115 | 45.724 | 30.422 | 64.774 | 1.00 | 27.56 | 6 |
| ATOM | 908 | O | GLU A 115 | 46.173 | 30.006 | 65.837 | 1.00 | 25.98 | 8 |
| ATOM | 909 | N | GLU A 116 | 45.267 | 31.660 | 64.615 | 1.00 | 31.19 | 7 |
| ATOM | 910 | CA | GLU A 116 | 45.282 | 32.631 | 65.705 | 1.00 | 35.80 | 6 |
| ATOM | 911 | CB | GLU A 116 | 44.676 | 33.959 | 65.237 | 1.00 | 36.91 | 6 |
| ATOM | 912 | CG | GLU A 116 | 45.434 | 34.605 | 64.069 | 1.00 | 41.14 | 6 |
| ATOM | 913 | CD | GLU A 116 | 46.872 | 34.982 | 64.420 | 1.00 | 43.09 | 6 |
| ATOM | 914 | OE1 | GLU A 116 | 47.072 | 35.886 | 65.267 | 1.00 | 43.42 | 8 |
| ATOM | 915 | OE2 | GLU A 116 | 47.802 | 34.369 | 63.849 | 1.00 | 41.76 | 8 |
| ATOM | 916 | C | GLU A 116 | 44.543 | 32.131 | 66.947 | 1.00 | 35.11 | 6 |
| ATOM | 917 | O | GLU A 116 | 45.054 | 32.228 | 68.061 | 1.00 | 37.26 | 8 |
| ATOM | 918 | N | PHE A 117 | 43.343 | 31.598 | 66.761 | 1.00 | 34.30 | 7 |
| ATOM | 919 | CA | PHE A 117 | 42.577 | 31.096 | 67.893 | 1.00 | 34.44 | 6 |
| ATOM | 920 | CB | PHE A 117 | 41.300 | 30.399 | 67.415 | 1.00 | 35.45 | 6 |
| ATOM | 921 | CG | PHE A 117 | 40.383 | 29.979 | 68.533 | 1.00 | 37.14 | 6 |
| ATOM | 922 | CD1 | PHE A 117 | 39.705 | 30.930 | 69.290 | 1.00 | 35.80 | 6 |
| ATOM | 923 | CD2 | PHE A 117 | 40.196 | 28.630 | 68.832 | 1.00 | 41.05 | 6 |
| ATOM | 924 | CE1 | PHE A 117 | 38.853 | 30.549 | 70.323 | 1.00 | 38.08 | 6 |

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Figure 17-15

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 925 | CE2 | PHE | A | 117 | 39.338 | 28.234 | 69.874 | 1.00 | 40.44 | 6 |
| ATOM | 926 | CZ | PHE | A | 117 | 38.668 | 29.198 | 70.617 | 1.00 | 38.64 | 6 |
| ATOM | 927 | C | PHE | A | 117 | 43.424 | 30.094 | 68.669 | 1.00 | 34.24 | 6 |
| ATOM | 928 | O | PHE | A | 117 | 43.490 | 30.136 | 69.898 | 1.00 | 33.54 | 8 |
| ATOM | 929 | N | LEU | A | 118 | 44.069 | 29.194 | 67.933 | 1.00 | 33.14 | 7 |
| ATOM | 930 | CA | LEU | A | 118 | 44.898 | 28.158 | 68.523 | 1.00 | 32.62 | 6 |
| ATOM | 931 | CB | LEU | A | 118 | 45.155 | 27.056 | 67.488 | 1.00 | 30.59 | 6 |
| ATOM | 932 | CG | LEU | A | 118 | 43.900 | 26.297 | 67.038 | 1.00 | 27.87 | 6 |
| ATOM | 933 | CD1 | LEU | A | 118 | 44.244 | 25.232 | 65.996 | 1.00 | 20.81 | 6 |
| ATOM | 934 | CD2 | LEU | A | 118 | 43.259 | 25.662 | 68.257 | 1.00 | 28.37 | 6 |
| ATOM | 935 | C | LEU | A | 118 | 46.216 | 28.696 | 69.084 | 1.00 | 34.37 | 6 |
| ATOM | 936 | O | LEU | A | 118 | 46.983 | 27.964 | 69.708 | 1.00 | 36.15 | 8 |
| ATOM | 937 | N | LYS | A | 119 | 46.481 | 29.974 | 68.843 | 1.00 | 34.75 | 7 |
| ATOM | 938 | CA | LYS | A | 119 | 47.679 | 30.609 | 69.365 | 1.00 | 34.34 | 6 |
| ATOM | 939 | CB | LYS | A | 119 | 48.143 | 31.739 | 68.448 | 1.00 | 33.52 | 6 |
| ATOM | 940 | CG | LYS | A | 119 | 48.614 | 31.270 | 67.100 | 1.00 | 37.98 | 6 |
| ATOM | 941 | CD | LYS | A | 119 | 49.111 | 32.430 | 66.263 | 1.00 | 43.40 | 6 |
| ATOM | 942 | CE | LYS | A | 119 | 49.691 | 31.928 | 64.949 | 1.00 | 46.52 | 6 |
| ATOM | 943 | NZ | LYS | A | 119 | 50.167 | 33.050 | 64.092 | 1.00 | 51.48 | 7 |
| ATOM | 944 | C | LYS | A | 119 | 47.273 | 31.191 | 70.705 | 1.00 | 34.85 | 6 |
| ATOM | 945 | O | LYS | A | 119 | 48.112 | 31.465 | 71.562 | 1.00 | 38.12 | 8 |
| ATOM | 946 | N | GLY | A | 120 | 45.967 | 31.372 | 70.869 | 1.00 | 34.15 | 7 |
| ATOM | 947 | CA | GLY | A | 120 | 45.431 | 31.927 | 72.094 | 1.00 | 36.25 | 6 |
| ATOM | 948 | C | GLY | A | 120 | 44.860 | 33.310 | 71.851 | 1.00 | 39.02 | 6 |
| ATOM | 949 | O | GLY | A | 120 | 44.640 | 34.072 | 72.796 | 1.00 | 40.23 | 8 |
| ATOM | 950 | N | ASN | A | 121 | 44.619 | 33.644 | 70.586 | 1.00 | 38.48 | 7 |
| ATOM | 951 | CA | ASN | A | 121 | 44.079 | 34.956 | 70.247 | 1.00 | 37.47 | 6 |
| ATOM | 952 | CB | ASN | A | 121 | 44.928 | 35.624 | 69.170 | 1.00 | 39.57 | 6 |
| ATOM | 953 | CG | ASN | A | 121 | 46.340 | 35.871 | 69.622 | 1.00 | 41.81 | 6 |
| ATOM | 954 | OD1 | ASN | A | 121 | 47.078 | 34.938 | 69.926 | 1.00 | 47.67 | 8 |
| ATOM | 955 | ND2 | ASN | A | 121 | 46.727 | 37.134 | 69.675 | 1.00 | 43.63 | 7 |
| ATOM | 956 | C | ASN | A | 121 | 42.637 | 34.893 | 69.772 | 1.00 | 36.59 | 6 |
| ATOM | 957 | O | ASN | A | 121 | 42.037 | 33.818 | 69.704 | 1.00 | 34.08 | 8 |
| ATOM | 958 | N | VAL | A | 122 | 42.092 | 36.061 | 69.446 | 1.00 | 33.53 | 7 |
| ATOM | 959 | CA | VAL | A | 122 | 40.720 | 36.166 | 68.976 | 1.00 | 34.77 | 6 |
| ATOM | 960 | CB | VAL | A | 122 | 39.861 | 37.064 | 69.898 | 1.00 | 38.20 | 6 |
| ATOM | 961 | CG1 | VAL | A | 122 | 38.418 | 37.096 | 69.388 | 1.00 | 37.55 | 6 |
| ATOM | 962 | CG2 | VAL | A | 122 | 39.918 | 36.553 | 71.342 | 1.00 | 37.77 | 6 |
| ATOM | 963 | C | VAL | A | 122 | 40.731 | 36.781 | 67.596 | 1.00 | 31.08 | 6 |
| ATOM | 964 | O | VAL | A | 122 | 40.991 | 37.967 | 67.441 | 1.00 | 34.19 | 8 |
| ATOM | 965 | N | ALA | A | 123 | 40.451 | 35.975 | 66.588 | 1.00 | 31.14 | 7 |
| ATOM | 966 | CA | ALA | A | 123 | 40.451 | 36.476 | 65.231 | 1.00 | 30.26 | 6 |
| ATOM | 967 | CB | ALA | A | 123 | 41.307 | 35.588 | 64.327 | 1.00 | 32.14 | 6 |
| ATOM | 968 | C | ALA | A | 123 | 39.038 | 36.533 | 64.716 | 1.00 | 28.26 | 6 |
| ATOM | 969 | O | ALA | A | 123 | 38.132 | 35.924 | 65.281 | 1.00 | 29.28 | 8 |
| ATOM | 970 | N | PHE | A | 124 | 38.875 | 37.276 | 63.631 | 1.00 | 28.70 | 7 |
| ATOM | 971 | CA | PHE | A | 124 | 37.601 | 37.475 | 62.976 | 1.00 | 28.38 | 6 |
| ATOM | 972 | CB | PHE | A | 124 | 36.920 | 38.713 | 63.563 | 1.00 | 29.16 | 6 |
| ATOM | 973 | CG | PHE | A | 124 | 35.645 | 39.099 | 62.874 | 1.00 | 31.20 | 6 |
| ATOM | 974 | CD1 | PHE | A | 124 | 34.679 | 38.139 | 62.564 | 1.00 | 32.00 | 6 |
| ATOM | 975 | CD2 | PHE | A | 124 | 35.378 | 40.435 | 62.579 | 1.00 | 29.53 | 6 |
| ATOM | 976 | CE1 | PHE | A | 124 | 33.463 | 38.510 | 61.973 | 1.00 | 30.74 | 6 |
| ATOM | 977 | CE2 | PHE | A | 124 | 34.165 | 40.813 | 61.988 | 1.00 | 27.45 | 6 |
| ATOM | 978 | CZ | PHE | A | 124 | 33.207 | 39.847 | 61.686 | 1.00 | 28.72 | 6 |
| ATOM | 979 | C | PHE | A | 124 | 37.880 | 37.671 | 61.496 | 1.00 | 30.19 | 6 |
| ATOM | 980 | O | PHE | A | 124 | 38.427 | 38.695 | 61.095 | 1.00 | 32.10 | 8 |
| ATOM | 981 | N | ASN | A | 125 | 37.545 | 36.663 | 60.696 | 1.00 | 32.16 | 7 |
| ATOM | 982 | CA | ASN | A | 125 | 37.731 | 36.728 | 59.251 | 1.00 | 30.10 | 6 |
| ATOM | 983 | CB | ASN | A | 125 | 38.247 | 35.393 | 58.712 | 1.00 | 32.02 | 6 |
| ATOM | 984 | CG | ASN | A | 125 | 38.281 | 35.360 | 57.195 | 1.00 | 33.79 | 6 |
| ATOM | 985 | OD1 | ASN | A | 125 | 38.754 | 36.306 | 56.556 | 1.00 | 31.85 | 8 |
| ATOM | 986 | ND2 | ASN | A | 125 | 37.790 | 34.268 | 56.609 | 1.00 | 30.51 | 7 |
| ATOM | 987 | C | ASN | A | 125 | 36.403 | 37.083 | 58.584 | 1.00 | 29.80 | 6 |
| ATOM | 988 | O | ASN | A | 125 | 35.626 | 36.206 | 58.179 | 1.00 | 27.24 | 8 |
| ATOM | 989 | N | PRO | A | 126 | 36.135 | 38.386 | 58.451 | 1.00 | 28.25 | 7 |
| ATOM | 990 | CD | PRO | A | 126 | 36.997 | 39.516 | 58.833 | 1.00 | 29.22 | 6 |

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Figure 17-16

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| ATOM | 991 | CA | PRO | A | 126 | 34.909 | 38.891 | 57.844 | 1.00 | 27.92 | 6 |
| ATOM | 992 | CB | PRO | A | 126 | 35.139 | 40.407 | 57.856 | 1.00 | 29.07 | 6 |
| ATOM | 993 | CG | PRO | A | 126 | 36.649 | 40.520 | 57.775 | 1.00 | 26.54 | 6 |
| ATOM | 994 | C | PRO | A | 126 | 34.651 | 38.339 | 56.448 | 1.00 | 27.54 | 6 |
| ATOM | 995 | O | PRO | A | 126 | 33.532 | 38.402 | 55.949 | 1.00 | 28.66 | 8 |
| ATOM | 996 | N | ALA | A | 127 | 35.687 | 37.795 | 55.820 | 1.00 | 26.99 | 7 |
| ATOM | 997 | CA | ALA | A | 127 | 35.548 | 37.244 | 54.477 | 1.00 | 26.54 | 6 |
| ATOM | 998 | CB | ALA | A | 127 | 36.822 | 37.505 | 53.684 | 1.00 | 22.43 | 6 |
| ATOM | 999 | C | ALA | A | 127 | 35.225 | 35.744 | 54.480 | 1.00 | 27.38 | 6 |
| ATOM | 1000 | O | ALA | A | 127 | 35.038 | 35.140 | 53.423 | 1.00 | 29.04 | 8 |
| ATOM | 1001 | N | GLY | A | 128 | 35.166 | 35.142 | 55.663 | 1.00 | 26.97 | 7 |
| ATOM | 1002 | CA | GLY | A | 128 | 34.874 | 33.724 | 55.737 | 1.00 | 25.65 | 6 |
| ATOM | 1003 | C | GLY | A | 128 | 33.389 | 33.486 | 55.880 | 1.00 | 26.17 | 6 |
| ATOM | 1004 | O | GLY | A | 128 | 32.600 | 34.428 | 55.804 | 1.00 | 27.39 | 8 |
| ATOM | 1005 | N | GLY | A | 129 | 32.998 | 32.234 | 56.083 | 1.00 | 23.87 | 7 |
| ATOM | 1006 | CA | GLY | A | 129 | 31.588 | 31.936 | 56.236 | 1.00 | 25.17 | 6 |
| ATOM | 1007 | C | GLY | A | 129 | 30.847 | 31.674 | 54.937 | 1.00 | 25.88 | 6 |
| ATOM | 1008 | O | GLY | A | 129 | 29.643 | 31.908 | 54.848 | 1.00 | 25.07 | 8 |
| ATOM | 1009 | N | MET | A | 130 | 31.566 | 31.198 | 53.927 | 1.00 | 25.69 | 7 |
| ATOM | 1010 | CA | MET | A | 130 | 30.981 | 30.872 | 52.622 | 1.00 | 26.48 | 6 |
| ATOM | 1011 | CB | MET | A | 130 | 32.103 | 30.907 | 51.567 | 1.00 | 28.53 | 6 |
| ATOM | 1012 | CG | MET | A | 130 | 32.795 | 32.288 | 51.467 | 1.00 | 26.54 | 6 |
| ATOM | 1013 | SD | MET | A | 130 | 34.413 | 32.366 | 50.613 | 1.00 | 26.29 | 16 |
| ATOM | 1014 | CE | MET | A | 130 | 34.080 | 31.512 | 49.062 | 1.00 | 25.85 | 6 |
| ATOM | 1015 | C | MET | A | 130 | 30.355 | 29.463 | 52.768 | 1.00 | 24.47 | 6 |
| ATOM | 1016 | O | MET | A | 130 | 30.761 | 28.502 | 52.113 | 1.00 | 17.67 | 8 |
| ATOM | 1017 | N | HIS | A | 131 | 29.347 | 29.389 | 53.636 | 1.00 | 23.28 | 7 |
| ATOM | 1018 | CA | HIS | A | 131 | 28.647 | 28.161 | 54.019 | 1.00 | 26.33 | 6 |
| ATOM | 1019 | CB | HIS | A | 131 | 27.685 | 28.485 | 55.180 | 1.00 | 26.98 | 6 |
| ATOM | 1020 | CG | HIS | A | 131 | 26.663 | 29.540 | 54.862 | 1.00 | 28.50 | 6 |
| ATOM | 1021 | CD2 | HIS | A | 131 | 26.225 | 30.030 | 53.677 | 1.00 | 28.65 | 6 |
| ATOM | 1022 | ND1 | HIS | A | 131 | 25.906 | 30.166 | 55.831 | 1.00 | 33.04 | 7 |
| ATOM | 1023 | CE1 | HIS | A | 131 | 25.051 | 30.995 | 55.259 | 1.00 | 27.75 | 6 |
| ATOM | 1024 | NE2 | HIS | A | 131 | 25.224 | 30.932 | 53.952 | 1.00 | 26.97 | 7 |
| ATOM | 1025 | C | HIS | A | 131 | 27.917 | 27.284 | 53.017 | 1.00 | 28.44 | 6 |
| ATOM | 1026 | O | HIS | A | 131 | 27.434 | 26.214 | 53.390 | 1.00 | 31.15 | 3 |
| ATOM | 1027 | N | HIS | A | 132 | 27.861 | 27.694 | 51.756 | 1.00 | 30.64 | 7 |
| ATOM | 1028 | CA | HIS | A | 132 | 27.111 | 26.938 | 50.746 | 1.00 | 28.71 | 6 |
| ATOM | 1029 | CB | HIS | A | 132 | 26.321 | 27.941 | 49.890 | 1.00 | 27.21 | 6 |
| ATOM | 1030 | CG | HIS | A | 132 | 25.408 | 28.819 | 50.693 | 1.00 | 28.83 | 6 |
| ATOM | 1031 | CD2 | HIS | A | 132 | 25.111 | 30.137 | 50.578 | 1.00 | 28.92 | 6 |
| ATOM | 1032 | ND1 | HIS | A | 132 | 24.686 | 28.360 | 51.773 | 1.00 | 31.80 | 7 |
| ATOM | 1033 | CE1 | HIS | A | 132 | 23.981 | 29.353 | 52.285 | 1.00 | 29.95 | 6 |
| ATOM | 1034 | NE2 | HIS | A | 132 | 24.222 | 30.443 | 51.579 | 1.00 | 28.21 | 7 |
| ATOM | 1035 | C | HIS | A | 132 | 27.889 | 25.970 | 49.851 | 1.00 | 28.51 | 6 |
| ATOM | 1036 | O | HIS | A | 132 | 27.399 | 24.775 | 49.533 | 1.00 | 23.44 | 8 |
| ATOM | 1037 | N | ALA | A | 133 | 29.093 | 26.379 | 49.455 | 1.00 | 27.94 | 7 |
| ATOM | 1038 | CA | ALA | A | 133 | 29.958 | 25.386 | 48.579 | 1.00 | 26.99 | 6 |
| ATOM | 1039 | CB | ALA | A | 133 | 31.295 | 26.303 | 48.392 | 1.00 | 21.87 | 6 |
| ATOM | 1040 | C | ALA | A | 133 | 30.199 | 24.164 | 49.078 | 1.00 | 26.69 | 6 |
| ATOM | 1041 | O | ALA | A | 133 | 30.703 | 23.973 | 50.182 | 1.00 | 28.25 | 8 |
| ATOM | 1042 | N | PHE | A | 134 | 29.850 | 23.174 | 48.255 | 1.00 | 26.73 | 7 |
| ATOM | 1043 | CA | PHE | A | 134 | 30.046 | 21.773 | 48.615 | 1.00 | 25.04 | 6 |
| ATOM | 1044 | CB | PHE | A | 134 | 29.070 | 20.855 | 47.875 | 1.00 | 19.20 | 6 |
| ATOM | 1045 | CG | PHE | A | 134 | 27.629 | 21.199 | 48.100 | 1.00 | 15.75 | 6 |
| ATOM | 1046 | CD1 | PHE | A | 134 | 26.929 | 21.960 | 47.169 | 1.00 | 14.83 | 6 |
| ATOM | 1047 | CD2 | PHE | A | 134 | 26.985 | 20.814 | 49.273 | 1.00 | 14.03 | 6 |
| ATOM | 1048 | CE1 | PHE | A | 134 | 25.614 | 22.336 | 47.404 | 1.00 | 14.84 | 6 |
| ATOM | 1049 | CE2 | PHE | A | 134 | 25.670 | 21.184 | 49.519 | 1.00 | 12.07 | 6 |
| ATOM | 1050 | CZ | PHE | A | 134 | 24.985 | 21.949 | 48.581 | 1.00 | 14.59 | 6 |
| ATOM | 1051 | C | PHE | A | 134 | 31.460 | 21.310 | 48.319 | 1.00 | 29.48 | 6 |
| ATOM | 1052 | O | PHE | A | 134 | 32.291 | 22.066 | 47.822 | 1.00 | 33.19 | 8 |
| ATOM | 1053 | N | LYS | A | 135 | 31.713 | 20.045 | 48.620 | 1.00 | 31.52 | 7 |
| ATOM | 1054 | CA | LYS | A | 135 | 33.012 | 19.427 | 48.427 | 1.00 | 29.15 | 6 |
| ATOM | 1055 | CB | LYS | A | 135 | 32.923 | 17.971 | 48.885 | 1.00 | 29.45 | 6 |
| ATOM | 1056 | CG | LYS | A | 135 | 34.152 | 17.131 | 48.638 | 1.00 | 32.46 | 6 |

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Figure 17-17

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| ATOM | 1057 | CD | LYS | A | 135 | 33.965 | 15.734 | 49.221 | 1.00 | 29.67 | 6 |
| ATOM | 1058 | CE | LYS | A | 135 | 34.234 | 15.703 | 50.716 | 1.00 | 30.09 | 6 |
| ATOM | 1059 | NZ | LYS | A | 135 | 35.679 | 15.973 | 51.001 | 1.00 | 26.25 | 7 |
| ATOM | 1060 | C | LYS | A | 135 | 33.513 | 19.516 | 46.993 | 1.00 | 30.22 | 6 |
| ATOM | 1061 | O | LYS | A | 135 | 34.714 | 19.672 | 46.763 | 1.00 | 30.00 | 8 |
| ATOM | 1062 | N | SER | A | 136 | 32.600 | 19.434 | 46.028 | 1.00 | 31.69 | 7 |
| ATOM | 1063 | CA | SER | A | 136 | 32.995 | 19.489 | 44.619 | 1.00 | 32.88 | 6 |
| ATOM | 1064 | CB | SER | A | 136 | 33.038 | 18.077 | 44.040 | 1.00 | 31.41 | 6 |
| ATOM | 1065 | OG | SER | A | 136 | 33.882 | 17.241 | 44.810 | 1.00 | 35.41 | 8 |
| ATOM | 1066 | C | SER | A | 136 | 32.097 | 20.347 | 43.727 | 1.00 | 33.55 | 6 |
| ATOM | 1067 | O | SER | A | 136 | 31.921 | 20.031 | 42.553 | 1.00 | 36.11 | 8 |
| ATOM | 1068 | N | ARG | A | 137 | 31.536 | 21.425 | 44.262 | 1.00 | 30.61 | 7 |
| ATOM | 1069 | CA | ARG | A | 137 | 30.664 | 22.272 | 43.459 | 1.00 | 32.28 | 6 |
| ATOM | 1070 | CB | ARG | A | 137 | 29.324 | 21.554 | 43.202 | 1.00 | 35.91 | 6 |
| ATOM | 1071 | CG | ARG | A | 137 | 28.224 | 22.458 | 42.627 | 1.00 | 43.90 | 6 |
| ATOM | 1072 | CD | ARG | A | 137 | 26.819 | 21.836 | 42.751 | 1.00 | 48.28 | 6 |
| ATOM | 1073 | NE | ARG | A | 137 | 26.571 | 20.767 | 41.787 | 1.00 | 53.38 | 7 |
| ATOM | 1074 | CZ | ARG | A | 137 | 26.150 | 20.960 | 40.538 | 1.00 | 55.30 | 6 |
| ATOM | 1075 | NH1 | ARG | A | 137 | 25.921 | 22.185 | 40.090 | 1.00 | 54.06 | 7 |
| ATOM | 1076 | NH2 | ARG | A | 137 | 25.969 | 19.922 | 39.728 | 1.00 | 58.96 | 7 |
| ATOM | 1077 | C | ARG | A | 137 | 30.405 | 23.631 | 44.113 | 1.00 | 30.24 | 6 |
| ATOM | 1078 | O | ARG | A | 137 | 30.380 | 23.748 | 45.338 | 1.00 | 23.11 | 8 |
| ATOM | 1079 | N | ALA | A | 138 | 30.219 | 24.653 | 43.279 | 1.00 | 27.33 | 7 |
| ATOM | 1080 | CA | ALA | A | 138 | 29.944 | 26.000 | 43.757 | 1.00 | 27.36 | 6 |
| ATOM | 1081 | CB | ALA | A | 138 | 30.149 | 26.997 | 42.645 | 1.00 | 27.57 | 6 |
| ATOM | 1082 | C | ALA | A | 138 | 28.496 | 26.003 | 44.213 | 1.00 | 26.45 | 6 |
| ATOM | 1083 | O | ALA | A | 138 | 27.747 | 25.083 | 43.865 | 1.00 | 27.30 | 8 |
| ATOM | 1084 | N | ASN | A | 139 | 28.090 | 27.021 | 44.975 | 1.00 | 22.47 | 7 |
| ATOM | 1085 | CA | ASN | A | 139 | 26.711 | 27.063 | 45.471 | 1.00 | 23.85 | 6 |
| ATOM | 1086 | CB | ASN | A | 139 | 26.406 | 25.738 | 46.218 | 1.00 | 16.82 | 6 |
| ATOM | 1087 | CG | ASN | A | 139 | 25.040 | 25.718 | 46.900 | 1.00 | 14.45 | 6 |
| ATOM | 1088 | OD1 | ASN | A | 139 | 24.019 | 26.084 | 46.319 | 1.00 | 13.39 | 8 |
| ATOM | 1089 | ND2 | ASN | A | 139 | 25.018 | 25.249 | 48.139 | 1.00 | 20.08 | 7 |
| ATOM | 1090 | C | ASN | A | 139 | 26.444 | 28.277 | 46.368 | 1.00 | 26.09 | 6 |
| ATOM | 1091 | O | ASN | A | 139 | 27.239 | 28.600 | 47.260 | 1.00 | 27.50 | 8 |
| ATOM | 1092 | N | GLY | A | 140 | 25.326 | 28.954 | 46.114 | 1.00 | 24.83 | 7 |
| ATOM | 1093 | CA | GLY | A | 140 | 24.965 | 30.106 | 46.916 | 1.00 | 22.24 | 6 |
| ATOM | 1094 | C | GLY | A | 140 | 25.991 | 31.211 | 46.890 | 1.00 | 22.35 | 6 |
| ATOM | 1095 | O | GLY | A | 140 | 26.256 | 31.843 | 47.910 | 1.00 | 23.50 | 8 |
| ATOM | 1096 | N | PHE | A | 141 | 26.570 | 31.437 | 45.717 | 1.00 | 25.60 | 7 |
| ATOM | 1097 | CA | PHE | A | 141 | 27.582 | 32.476 | 45.518 | 1.00 | 26.47 | 6 |
| ATOM | 1098 | CB | PHE | A | 141 | 27.204 | 33.765 | 46.258 | 1.00 | 28.05 | 6 |
| ATOM | 1099 | CG | PHE | A | 141 | 25.925 | 34.391 | 45.792 | 1.00 | 28.61 | 6 |
| ATOM | 1100 | CD1 | PHE | A | 141 | 25.352 | 35.428 | 46.518 | 1.00 | 30.74 | 6 |
| ATOM | 1101 | CD2 | PHE | A | 141 | 25.312 | 33.975 | 44.620 | 1.00 | 29.10 | 6 |
| A OM | 1102 | CE1 | PHE | A | 141 | 24.193 | 36.044 | 46.087 | 1.00 | 29.33 | 6 |
| ATOM | 1103 | CE2 | PHE | A | 141 | 24.150 | 34.583 | 44.177 | 1.00 | 31.03 | 6 |
| ATOM | 1104 | CZ | PHE | A | 141 | 23.589 | 35.621 | 44.912 | 1.00 | 32.59 | 6 |
| ATOM | 1105 | C | PHE | A | 141 | 28.954 | 32.038 | 45.991 | 1.00 | 24.63 | 6 |
| ATOM | 1106 | O | PHE | A | 141 | 29.938 | 32.727 | 45.733 | 1.00 | 29.72 | 8 |
| ATOM | 1107 | N | CYS | A | 142 | 29.025 | 30.897 | 46.667 | 1.00 | 21.11 | 7 |
| ATOM | 1108 | CA | CYS | A | 142 | 30.296 | 30.399 | 47.192 | 1.00 | 22.30 | 6 |
| ATOM | 1109 | CB | CYS | A | 142 | 30.062 | 29.787 | 48.567 | 1.00 | 21.31 | 6 |
| ATOM | 1110 | SG | CYS | A | 142 | 28.943 | 30.748 | 49.582 | 1.00 | 22.93 | 16 |
| ATOM | 1111 | C | CYS | A | 142 | 31.017 | 29.366 | 46.326 | 1.00 | 22.13 | 6 |
| ATOM | 1112 | O | CYS | A | 142 | 30.408 | 28.389 | 45.878 | 1.00 | 22.97 | 8 |
| ATOM | 1113 | N | TYR | A | 143 | 32.317 | 29.573 | 46.111 | 1.00 | 23.09 | 7 |
| ATOM | 1114 | CA | TYR | A | 143 | 33.129 | 28.632 | 45.335 | 1.00 | 23.05 | 6 |
| ATOM | 1115 | CB | TYR | A | 143 | 34.063 | 29.365 | 44.375 | 1.00 | 21.60 | 6 |
| ATOM | 1116 | CG | TYR | A | 143 | 33.377 | 30.379 | 43.487 | 1.00 | 24.09 | 6 |
| ATOM | 1117 | CD1 | TYR | A | 143 | 32.969 | 31.609 | 43.999 | 1.00 | 23.29 | 6 |
| ATOM | 1118 | CE1 | TYR | A | 143 | 32.365 | 32.555 | 43.199 | 1.00 | 23.26 | 6 |
| ATOM | 1119 | CD2 | TYR | A | 143 | 33.154 | 30.117 | 42.135 | 1.00 | 22.52 | 6 |
| ATOM | 1120 | CE2 | TYR | A | 143 | 32.544 | 31.061 | 41.317 | 1.00 | 24.82 | 6 |
| ATOM | 1121 | CZ | TYR | A | 143 | 32.153 | 32.281 | 41.857 | 1.00 | 27.55 | 6 |
| ATOM | 1122 | OH | TYR | A | 143 | 31.553 | 33.241 | 41.064 | 1.00 | 32.35 | 8 |

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Figure 17-18

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1123 | C | TYR | A | 143 | 33.960 | 27.766 | 46.290 | 1.00 | 24.22 | 6 |
| ATOM | 1124 | O | TYR | A | 143 | 34.266 | 26.606 | 45.998 | 1.00 | 24.58 | 8 |
| ATOM | 1125 | N | ILE | A | 144 | 34.327 | 28.329 | 47.437 | 1.00 | 23.83 | 7 |
| ATOM | 1126 | CA | ILE | A | 144 | 35.086 | 27.566 | 48.425 | 1.00 | 20.24 | 6 |
| ATOM | 1127 | CB | ILE | A | 144 | 36.547 | 27.982 | 48.453 | 1.00 | 17.27 | 6 |
| ATOM | 1128 | CG2 | ILE | A | 144 | 37.231 | 27.354 | 49.662 | 1.00 | 11.03 | 6 |
| ATOM | 1129 | CG1 | ILE | A | 144 | 37.185 | 27.603 | 47.110 | 1.00 | 14.93 | 6 |
| ATOM | 1130 | CD1 | ILE | A | 144 | 38.601 | 28.028 | 46.946 | 1.00 | 19.68 | 6 |
| ATOM | 1131 | C | ILE | A | 144 | 34.495 | 27.703 | 49.815 | 1.00 | 21.77 | 6 |
| ATOM | 1132 | O | ILE | A | 144 | 34.288 | 28.811 | 50.318 | 1.00 | 21.19 | 8 |
| ATOM | 1133 | N | ASN | A | 145 | 34.212 | 26.555 | 50.424 | 1.00 | 23.00 | 7 |
| ATOM | 1134 | CA | ASN | A | 145 | 33.616 | 26.508 | 51.750 | 1.00 | 20.92 | 6 |
| ATOM | 1135 | CB | ASN | A | 145 | 32.902 | 25.170 | 51.935 | 1.00 | 17.08 | 6 |
| ATOM | 1136 | CG | ASN | A | 145 | 32.079 | 25.125 | 53.203 | 1.00 | 21.04 | 6 |
| ATOM | 1137 | OD1 | ASN | A | 145 | 32.549 | 25.508 | 54.276 | 1.00 | 20.97 | 8 |
| ATOM | 1138 | ND2 | ASN | A | 145 | 30.844 | 24.640 | 53.093 | 1.00 | 20.93 | 7 |
| ATOM | 1139 | C | ASN | A | 145 | 34.706 | 26.669 | 52.806 | 1.00 | 19.68 | 6 |
| ATOM | 1140 | O | ASN | A | 145 | 35.201 | 25.679 | 53.351 | 1.00 | 20.64 | 8 |
| ATOM | 1141 | N | ASN | A | 146 | 35.079 | 27.911 | 53.100 | 1.00 | 16.28 | 7 |
| ATOM | 1142 | CA | ASN | A | 146 | 36.123 | 28.143 | 54.088 | 1.00 | 19.34 | 6 |
| ATOM | 1143 | CB | ASN | A | 146 | 36.428 | 29.651 | 54.207 | 1.00 | 20.27 | 6 |
| ATOM | 1144 | CG | ASN | A | 146 | 35.292 | 30.444 | 54.795 | 1.00 | 18.05 | 6 |
| ATOM | 1145 | OD1 | ASN | A | 146 | 35.079 | 30.421 | 55.999 | 1.00 | 25.83 | 8 |
| ATOM | 1146 | ND2 | ASN | A | 146 | 34.552 | 31.149 | 53.948 | 1.00 | 16.04 | 7 |
| ATOM | 1147 | C | ASN | A | 146 | 35.775 | 27.504 | 55.443 | 1.00 | 20.48 | 6 |
| ATOM | 1148 | O | ASN | A | 146 | 36.663 | 27.027 | 56.151 | 1.00 | 19.88 | 8 |
| ATOM | 1149 | N | PRO | A | 147 | 34.482 | 27.485 | 55.819 | 1.00 | 19.38 | 7 |
| ATOM | 1150 | CD | PRO | A | 147 | 33.312 | 28.068 | 55.135 | 1.00 | 17.48 | 6 |
| ATOM | 1151 | CA | PRO | A | 147 | 34.058 | 26.877 | 57.087 | 1.00 | 22.25 | 6 |
| ATOM | 1152 | CB | PRO | A | 147 | 32.539 | 27.065 | 57.057 | 1.00 | 20.15 | 6 |
| ATOM | 1153 | CG | PRO | A | 147 | 32.407 | 28.378 | 56.305 | 1.00 | 20.81 | 6 |
| ATOM | 1154 | C | PRO | A | 147 | 34.443 | 25.383 | 57.188 | 1.00 | 26.89 | 6 |
| ATOM | 1155 | O | PRO | A | 147 | 35.066 | 24.954 | 58.169 | 1.00 | 29.10 | 8 |
| ATOM | 1156 | N | ALA | A | 148 | 34.070 | 24.596 | 56.176 | 1.00 | 25.88 | 7 |
| ATOM | 1157 | CA | ALA | A | 148 | 34.372 | 23.164 | 56.174 | 1.00 | 25.47 | 6 |
| ATOM | 1158 | CB | ALA | A | 148 | 33.670 | 22.468 | 55.009 | 1.00 | 21.84 | 6 |
| ATOM | 1159 | C | ALA | A | 148 | 35.870 | 22.916 | 56.100 | 1.00 | 25.94 | 6 |
| ATOM | 1160 | O | ALA | A | 148 | 36.382 | 21.971 | 56.701 | 1.00 | 27.19 | 8 |
| ATOM | 1161 | N | VAL | A | 149 | 36.574 | 23.756 | 55.349 | 1.00 | 26.11 | 7 |
| ATOM | 1162 | CA | VAL | A | 149 | 38.017 | 23.609 | 55.233 | 1.00 | 24.04 | 6 |
| ATOM | 1163 | CB | VAL | A | 149 | 38.622 | 24.663 | 54.267 | 1.00 | 26.16 | 6 |
| ATOM | 1164 | CG1 | VAL | A | 149 | 40.135 | 24.476 | 54.158 | 1.00 | 25.36 | 6 |
| ATOM | 1165 | CG2 | VAL | A | 149 | 37.970 | 24.544 | 52.886 | 1.00 | 26.81 | 6 |
| ATOM | 1166 | C | VAL | A | 149 | 38.516 | 23.870 | 56.640 | 1.00 | 23.57 | 6 |
| ATOM | 1167 | O | VAL | A | 149 | 39.453 | 23.228 | 57.122 | 1.00 | 19.75 | 8 |
| ATOM | 1168 | N | GLY | A | 150 | 37.850 | 24.815 | 57.299 | 1.00 | 22.20 | 7 |
| ATOM | 1169 | CA | GLY | A | 150 | 38.210 | 25.175 | 58.654 | 1.00 | 25.43 | 6 |
| ATOM | 1170 | C | GLY | A | 150 | 38.130 | 23.975 | 59.568 | 1.00 | 27.19 | 6 |
| ATOM | 1171 | O | GLY | A | 150 | 39.112 | 23.620 | 60.221 | 1.00 | 27.05 | 8 |
| ATOM | 1172 | N | ILE | A | 151 | 36.959 | 23.348 | 59.618 | 1.00 | 25.56 | 7 |
| ATOM | 1173 | CA | ILE | A | 151 | 36.775 | 22.176 | 60.457 | 1.00 | 28.24 | 6 |
| ATOM | 1174 | CB | ILE | A | 151 | 35.317 | 21.654 | 60.389 | 1.00 | 29.41 | 6 |
| ATOM | 1175 | CG2 | ILE | A | 151 | 35.251 | 20.215 | 60.869 | 1.00 | 26.02 | 6 |
| ATOM | 1176 | CG1 | ILE | A | 151 | 34.394 | 22.540 | 61.240 | 1.00 | 33.31 | 6 |
| ATOM | 1177 | CD1 | ILE | A | 151 | 34.255 | 23.967 | 60.759 | 1.00 | 36.83 | 6 |
| ATOM | 1178 | C | ILE | A | 151 | 37.723 | 21.039 | 60.075 | 1.00 | 29.32 | 6 |
| ATOM | 1179 | O | ILE | A | 151 | 38.340 | 20.420 | 60.947 | 1.00 | 29.08 | 8 |
| ATOM | 1180 | N | GLU | A | 152 | 37.843 | 20.769 | 58.778 | 1.00 | 29.91 | 7 |
| ATOM | 1181 | CA | GLU | A | 152 | 38.704 | 19.690 | 58.315 | 1.00 | 32.58 | 6 |
| ATOM | 1182 | CB | GLU | A | 152 | 38.575 | 19.526 | 56.802 | 1.00 | 35.07 | 6 |
| ATOM | 1183 | CG | GLU | A | 152 | 37.269 | 18.848 | 56.393 | 1.00 | 38.51 | 6 |
| ATOM | 1184 | CD | GLU | A | 152 | 37.120 | 17.440 | 56.987 | 1.00 | 41.41 | 6 |
| ATOM | 1185 | OE1 | GLU | A | 152 | 36.089 | 16.779 | 56.718 | 1.00 | 45.64 | 8 |
| ATOM | 1186 | OE2 | GLU | A | 152 | 38.030 | 16.992 | 57.723 | 1.00 | 40.09 | 8 |
| ATOM | 1187 | C | GLU | A | 152 | 40.145 | 19.903 | 58.721 | 1.00 | 32.97 | 6 |
| ATOM | 1188 | O | GLU | A | 152 | 40.879 | 18.946 | 58.978 | 1.00 | 30.15 | 8 |

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Figure 17-19

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1189 | N | TYR | A | 153 | 40.541 | 21.170 | 58.765 | 1.00 | 33.90 | 7 |
| ATOM | 1190 | CA | TYR | A | 153 | 41.875 | 21.563 | 59.193 | 1.00 | 32.04 | 6 |
| ATOM | 1191 | CB | TYR | A | 153 | 42.019 | 23.074 | 59.058 | 1.00 | 34.88 | 6 |
| ATOM | 1192 | CG | TYR | A | 153 | 43.280 | 23.667 | 59.639 | 1.00 | 38.03 | 6 |
| ATOM | 1193 | CD1 | TYR | A | 153 | 44.498 | 23.611 | 58.948 | 1.00 | 42.34 | 6 |
| ATOM | 1194 | CE1 | TYR | A | 153 | 45.658 | 24.207 | 59.475 | 1.00 | 43.38 | 6 |
| ATOM | 1195 | CD2 | TYR | A | 153 | 43.250 | 24.321 | 60.869 | 1.00 | 37.19 | 6 |
| ATOM | 1196 | CE2 | TYR | A | 153 | 44.387 | 24.913 | 61.401 | 1.00 | 41.09 | 6 |
| ATOM | 1197 | CZ | TYR | A | 153 | 45.587 | 24.860 | 60.704 | 1.00 | 43.34 | 6 |
| ATOM | 1198 | OH | TYR | A | 153 | 46.696 | 25.480 | 61.241 | 1.00 | 44.86 | 8 |
| ATOM | 1199 | C | TYR | A | 153 | 41.919 | 21.168 | 60.667 | 1.00 | 32.59 | 6 |
| ATOM | 1200 | O | TYR | A | 153 | 42.867 | 20.518 | 61.120 | 1.00 | 32.24 | 8 |
| ATOM | 1201 | N | LEU | A | 154 | 40.869 | 21.556 | 61.397 | 1.00 | 30.10 | 7 |
| ATOM | 1202 | CA | LEU | A | 154 | 40.730 | 21.261 | 62.823 | 1.00 | 29.38 | 6 |
| ATOM | 1203 | CB | LEU | A | 154 | 39.443 | 21.889 | 63.378 | 1.00 | 28.60 | 6 |
| ATOM | 1204 | CG | LEU | A | 154 | 39.399 | 23.407 | 63.618 | 1.00 | 31.20 | 6 |
| ATOM | 1205 | CD1 | LEU | A | 154 | 37.991 | 23.833 | 64.041 | 1.00 | 28.53 | 6 |
| ATOM | 1206 | CD2 | LEU | A | 154 | 40.418 | 23.787 | 64.691 | 1.00 | 24.95 | 6 |
| ATOM | 1207 | C | LEU | A | 154 | 40.732 | 19.772 | 63.146 | 1.00 | 29.56 | 6 |
| ATOM | 1208 | O | LEU | A | 154 | 41.223 | 19.363 | 64.196 | 1.00 | 28.36 | 8 |
| ATOM | 1209 | N | ARG | A | 155 | 40.174 | 18.958 | 62.256 | 1.00 | 31.95 | 7 |
| ATOM | 1210 | CA | ARG | A | 155 | 40.134 | 17.522 | 62.499 | 1.00 | 33.00 | 6 |
| ATOM | 1211 | CB | ARG | A | 155 | 39.127 | 16.847 | 61.561 | 1.00 | 33.13 | 6 |
| ATOM | 1212 | CG | ARG | A | 155 | 37.708 | 17.368 | 61.769 | 1.00 | 32.84 | 6 |
| ATOM | 1213 | CD | ARG | A | 155 | 36.678 | 16.719 | 60.863 | 1.00 | 32.92 | 6 |
| ATOM | 1214 | NE | ARG | A | 155 | 36.152 | 15.451 | 61.363 | 1.00 | 33.98 | 7 |
| ATOM | 1215 | CZ | ARG | A | 155 | 35.195 | 14.760 | 60.741 | 1.00 | 37.93 | 6 |
| ATOM | 1216 | NH1 | ARG | A | 155 | 34.671 | 15.216 | 59.605 | 1.00 | 38.39 | 7 |
| ATOM | 1217 | NH2 | ARG | A | 155 | 34.732 | 13.631 | 61.259 | 1.00 | 38.67 | 7 |
| ATOM | 1218 | C | ARG | A | 155 | 41.521 | 16.929 | 62.331 | 1.00 | 33.97 | 6 |
| ATOM | 1219 | O | ARG | A | 155 | 41.869 | 15.941 | 62.985 | 1.00 | 32.95 | 8 |
| ATOM | 1220 | N | LYS | A | 156 | 42.318 | 17.548 | 61.467 | 1.00 | 34.20 | 7 |
| ATOM | 1221 | CA | LYS | A | 156 | 43.679 | 17.081 | 61.243 | 1.00 | 36.32 | 6 |
| ATOM | 1222 | CB | LYS | A | 156 | 44.249 | 17.662 | 59.942 | 1.00 | 37.57 | 6 |
| ATOM | 1223 | CG | LYS | A | 156 | 45.673 | 17.187 | 59.638 | 1.00 | 40.32 | 6 |
| ATOM | 1224 | CD | LYS | A | 156 | 46.116 | 17.532 | 58.220 | 1.00 | 40.33 | 6 |
| ATOM | 1225 | CE | LYS | A | 156 | 45.180 | 16.909 | 57.184 | 1.00 | 41.27 | 6 |
| ATOM | 1226 | NZ | LYS | A | 156 | 45.015 | 15.435 | 57.364 | 1.00 | 37.92 | 7 |
| ATOM | 1227 | C | LYS | A | 156 | 44.539 | 17.501 | 62.428 | 1.00 | 36.17 | 6 |
| ATOM | 1228 | O | LYS | A | 156 | 45.582 | 16.905 | 62.699 | 1.00 | 34.53 | 8 |
| ATOM | 1229 | N | LYS | A | 157 | 44.093 | 18.537 | 63.132 | 1.00 | 36.71 | 7 |
| ATOM | 1230 | CA | LYS | A | 157 | 44.820 | 19.026 | 64.294 | 1.00 | 37.09 | 6 |
| ATOM | 1231 | CB | LYS | A | 157 | 44.495 | 20.501 | 64.566 | 1.00 | 37.02 | 6 |
| ATOM | 1232 | CG | LYS | A | 157 | 44.982 | 21.435 | 63.477 | 1.00 | 36.22 | 6 |
| ATOM | 1233 | CD | LYS | A | 157 | 46.468 | 21.231 | 63.239 | 1.00 | 37.91 | 6 |
| ATOM | 1234 | CE | LYS | A | 157 | 46.993 | 22.100 | 62.107 | 1.00 | 39.35 | 6 |
| ATOM | 1235 | NZ | LYS | A | 157 | 48.434 | 21.815 | 61.842 | 1.00 | 38.78 | 7 |
| ATOM | 1236 | C | LYS | A | 157 | 44.498 | 18.178 | 65.515 | 1.00 | 35.61 | 6 |
| ATOM | 1237 | O | LYS | A | 157 | 45.204 | 18.232 | 66.518 | 1.00 | 36.38 | 8 |
| ATOM | 1238 | N | GLY | A | 158 | 43.433 | 17.392 | 65.431 | 1.00 | 34.37 | 7 |
| ATOM | 1239 | CA | GLY | A | 158 | 43.097 | 16.537 | 66.552 | 1.00 | 38.08 | 6 |
| ATOM | 1240 | C | GLY | A | 158 | 41.782 | 16.781 | 67.267 | 1.00 | 38.78 | 6 |
| ATOM | 1241 | O | GLY | A | 158 | 41.460 | 16.053 | 68.208 | 1.00 | 41.07 | 8 |
| ATOM | 1242 | N | PHE | A | 159 | 41.023 | 17.791 | 66.855 | 1.00 | 36.75 | 7 |
| ATOM | 1243 | CA | PHE | A | 159 | 39.743 | 18.046 | 67.505 | 1.00 | 33.83 | 6 |
| ATOM | 1244 | CB | PHE | A | 159 | 39.246 | 19.459 | 67.213 | 1.00 | 32.65 | 6 |
| ATOM | 1245 | CG | PHE | A | 159 | 40.115 | 20.521 | 67.787 | 1.00 | 29.97 | 6 |
| ATOM | 1246 | CD1 | PHE | A | 159 | 41.404 | 20.724 | 67.297 | 1.00 | 30.20 | 6 |
| ATOM | 1247 | CD2 | PHE | A | 159 | 39.672 | 21.289 | 68.853 | 1.00 | 29.28 | 6 |
| ATOM | 1248 | CE1 | PHE | A | 159 | 42.241 | 21.680 | 67.862 | 1.00 | 28.96 | 6 |
| ATOM | 1249 | CE2 | PHE | A | 159 | 40.498 | 22.246 | 69.428 | 1.00 | 29.67 | 6 |
| ATOM | 1250 | CZ | PHE | A | 159 | 41.785 | 22.442 | 68.931 | 1.00 | 30.59 | 6 |
| ATOM | 1251 | C | PHE | A | 159 | 38.732 | 17.026 | 67.025 | 1.00 | 33.41 | 6 |
| ATOM | 1252 | O | PHE | A | 159 | 38.664 | 16.716 | 65.838 | 1.00 | 31.61 | 8 |
| ATOM | 1253 | N | LYS | A | 160 | 37.951 | 16.506 | 67.966 | 1.00 | 35.13 | 7 |
| ATOM | 1254 | CA | LYS | A | 160 | 36.947 | 15.493 | 67.677 | 1.00 | 35.39 | 6 |

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Figure 17-20

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1255 | CB | LYS | A | 160 | 37.342 | 14.198 | 68.389 | 1.00 | 36.43 | 6 |
| ATOM | 1256 | CG | LYS | A | 160 | 38.535 | 13.502 | 67.708 | 1.00 | 40.67 | 6 |
| ATOM | 1257 | CD | LYS | A | 160 | 39.312 | 12.538 | 68.615 | 1.00 | 44.68 | 6 |
| ATOM | 1258 | CE | LYS | A | 160 | 38.425 | 11.536 | 69.345 | 1.00 | 49.23 | 6 |
| ATOM | 1259 | NZ | LYS | A | 160 | 37.593 | 12.182 | 70.411 | 1.00 | 50.63 | 7 |
| ATOM | 1260 | C | LYS | A | 160 | 35.524 | 15.927 | 68.027 | 1.00 | 35.94 | 6 |
| ATOM | 1261 | O | LYS | A | 160 | 34.561 | 15.241 | 67.691 | 1.00 | 35.72 | 8 |
| ATOM | 1262 | N | ARG | A | 161 | 35.399 | 17.058 | 68.718 | 1.00 | 34.35 | 7 |
| ATOM | 1263 | CA | ARG | A | 161 | 34.091 | 17.618 | 69.044 | 1.00 | 34.95 | 6 |
| ATOM | 1264 | CB | ARG | A | 161 | 33.771 | 17.525 | 70.535 | 1.00 | 33.94 | 6 |
| ATOM | 1265 | CG | ARG | A | 161 | 33.427 | 16.132 | 70.992 | 1.00 | 38.25 | 6 |
| ATOM | 1266 | CD | ARG | A | 161 | 32.823 | 16.131 | 72.386 | 1.00 | 41.17 | 6 |
| ATOM | 1267 | NE | ARG | A | 161 | 33.719 | 16.722 | 73.378 | 1.00 | 47.64 | 7 |
| ATOM | 1268 | CZ | ARG | A | 161 | 34.912 | 16.233 | 73.705 | 1.00 | 47.92 | 6 |
| ATOM | 1269 | NH1 | ARG | A | 161 | 35.372 | 15.131 | 73.121 | 1.00 | 47.56 | 7 |
| ATOM | 1270 | NH2 | ARG | A | 161 | 35.648 | 16.858 | 74.616 | 1.00 | 46.95 | 7 |
| ATOM | 1271 | C | ARG | A | 161 | 34.113 | 19.076 | 68.598 | 1.00 | 34.58 | 6 |
| ATOM | 1272 | O | ARG | A | 161 | 34.468 | 19.980 | 69.357 | 1.00 | 33.77 | 8 |
| ATOM | 1273 | N | ILE | A | 162 | 33.741 | 19.280 | 67.341 | 1.00 | 31.74 | 7 |
| ATOM | 1274 | CA | ILE | A | 162 | 33.735 | 20.594 | 66.735 | 1.00 | 29.83 | 6 |
| ATOM | 1275 | CB | ILE | A | 162 | 34.429 | 20.542 | 65.362 | 1.00 | 29.96 | 6 |
| ATOM | 1276 | CG2 | ILE | A | 162 | 34.580 | 21.942 | 64.784 | 1.00 | 30.57 | 6 |
| ATOM | 1277 | CG1 | ILE | A | 162 | 35.801 | 19.891 | 65.522 | 1.00 | 28.81 | 6 |
| ATOM | 1278 | CD1 | ILE | A | 162 | 36.537 | 19.685 | 64.224 | 1.00 | 33.05 | 6 |
| ATOM | 1279 | C | ILE | A | 162 | 32.300 | 21.050 | 66.560 | 1.00 | 29.66 | 6 |
| ATOM | 1280 | O | ILE | A | 162 | 31.416 | 20.241 | 66.266 | 1.00 | 25.24 | 8 |
| ATOM | 1281 | N | LEU | A | 163 | 32.081 | 22.351 | 66.745 | 1.00 | 30.00 | 7 |
| ATOM | 1282 | CA | LEU | A | 163 | 30.754 | 22.945 | 66.617 | 1.00 | 30.48 | 6 |
| ATOM | 1283 | CB | LEU | A | 163 | 30.236 | 23.406 | 67.992 | 1.00 | 32.25 | 6 |
| ATOM | 1284 | CG | LEU | A | 163 | 28.934 | 24.229 | 68.044 | 1.00 | 31.21 | 6 |
| ATOM | 1285 | CD1 | LEU | A | 163 | 27.804 | 23.494 | 67.326 | 1.00 | 31.58 | 6 |
| ATOM | 1286 | CD2 | LEU | A | 163 | 28.569 | 24.502 | 69.493 | 1.00 | 25.00 | 6 |
| ATOM | 1287 | C | LEU | A | 163 | 30.717 | 24.122 | 65.659 | 1.00 | 29.23 | 6 |
| ATOM | 1288 | O | LEU | A | 163 | 31.596 | 24.980 | 65.654 | 1.00 | 29.72 | 8 |
| ATOM | 1289 | N | TYR | A | 164 | 29.675 | 24.157 | 64.846 | 1.00 | 29.68 | 7 |
| ATOM | 1290 | CA | TYR | A | 164 | 29.500 | 25.244 | 63.899 | 1.00 | 29.89 | 6 |
| ATOM | 1291 | CB | TYR | A | 164 | 29.512 | 24.688 | 62.470 | 1.00 | 27.81 | 6 |
| ATOM | 1292 | CG | TYR | A | 164 | 29.377 | 25.742 | 61.399 | 1.00 | 27.79 | 6 |
| ATOM | 1293 | CD1 | TYR | A | 164 | 30.390 | 26.670 | 61.168 | 1.00 | 24.82 | 6 |
| ATOM | 1294 | CE1 | TYR | A | 164 | 30.247 | 27.655 | 60.198 | 1.00 | 24.51 | 6 |
| ATOM | 1295 | CD2 | TYR | A | 164 | 28.216 | 25.827 | 60.631 | 1.00 | 27.61 | 6 |
| ATOM | 1296 | CE2 | TYR | A | 164 | 28.065 | 26.808 | 59.662 | 1.00 | 25.67 | 6 |
| ATOM | 1297 | CZ | TYR | A | 164 | 29.078 | 27.718 | 59.451 | 1.00 | 25.63 | 6 |
| ATOM | 1298 | OH | TYR | A | 164 | 28.898 | 28.704 | 58.506 | 1.00 | 27.10 | 8 |
| ATOM | 1299 | C | TYR | A | 164 | 28.149 | 25.907 | 64.218 | 1.00 | 28.38 | 6 |
| ATOM | 1300 | O | TYR | A | 164 | 27.119 | 25.225 | 64.277 | 1.00 | 29.43 | 8 |
| ATOM | 1301 | N | ILE | A | 165 | 28.166 | 27.217 | 64.464 | 1.00 | 24.30 | 7 |
| ATOM | 1302 | CA | ILE | A | 165 | 26.941 | 27.969 | 64.754 | 1.00 | 22.93 | 6 |
| ATOM | 1303 | CB | ILE | A | 165 | 26.985 | 28.649 | 66.143 | 1.00 | 22.00 | 6 |
| ATOM | 1304 | CG2 | ILE | A | 165 | 25.765 | 29.559 | 66.312 | 1.00 | 16.15 | 6 |
| ATOM | 1305 | CG1 | ILE | A | 165 | 27.033 | 27.567 | 67.240 | 1.00 | 20.78 | 6 |
| ATOM | 1306 | CD1 | ILE | A | 165 | 27.185 | 28.101 | 68.650 | 1.00 | 15.49 | 6 |
| ATOM | 1307 | C | ILE | A | 165 | 26.784 | 29.010 | 63.657 | 1.00 | 24.45 | 6 |
| ATOM | 1308 | O | ILE | A | 165 | 27.605 | 29.921 | 63.506 | 1.00 | 23.17 | 8 |
| ATOM | 1309 | N | ASP | A | 166 | 25.709 | 28.871 | 62.895 | 1.00 | 24.20 | 7 |
| ATOM | 1310 | CA | ASP | A | 166 | 25.478 | 29.726 | 61.749 | 1.00 | 20.78 | 6 |
| ATOM | 1311 | CB | ASP | A | 166 | 25.314 | 28.809 | 60.548 | 1.00 | 17.64 | 6 |
| ATOM | 1312 | CG | ASP | A | 166 | 25.410 | 29.529 | 59.256 | 1.00 | 19.93 | 6 |
| ATOM | 1313 | OD1 | ASP | A | 166 | 24.536 | 30.391 | 59.004 | 1.00 | 20.20 | 8 |
| ATOM | 1314 | OD2 | ASP | A | 166 | 26.366 | 29.231 | 58.491 | 1.00 | 17.64 | 8 |
| ATOM | 1315 | C | ASP | A | 166 | 24.290 | 30.670 | 61.895 | 1.00 | 22.79 | 6 |
| ATOM | 1316 | O | ASP | A | 166 | 23.134 | 30.256 | 61.826 | 1.00 | 22.70 | 8 |
| ATOM | 1317 | N | LEU | A | 167 | 24.583 | 31.952 | 62.085 | 1.00 | 25.40 | 7 |
| ATOM | 1318 | CA | LEU | A | 167 | 23.536 | 32.954 | 62.250 | 1.00 | 25.76 | 6 |
| ATOM | 1319 | CB | LEU | A | 167 | 23.963 | 33.991 | 63.288 | 1.00 | 26.65 | 6 |
| ATOM | 1320 | CG | LEU | A | 167 | 24.364 | 33.463 | 64.674 | 1.00 | 26.75 | 6 |

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Figure 17-21

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| ATOM | 1321 | CD1 | LEU | A | 167 | 24.741 | 34.647 | 65.552 | 1.00 | 26.24 | 6 |
| ATOM | 1322 | CD2 | LEU | A | 167 | 23.225 | 32.661 | 65.302 | 1.00 | 23.45 | 6 |
| ATOM | 1323 | C | LEU | A | 167 | 23.162 | 33.660 | 60.951 | 1.00 | 26.37 | 6 |
| ATOM | 1324 | O | LEU | A | 167 | 22.386 | 34.613 | 60.971 | 1.00 | 25.95 | 8 |
| ATOM | 1325 | N | ASP | A | 168 | 23.726 | 33.208 | 59.828 | 1.00 | 29.66 | 7 |
| ATOM | 1326 | CA | ASP | A | 168 | 23.410 | 33.787 | 58.520 | 1.00 | 28.35 | 6 |
| ATOM | 1327 | CB | ASP | A | 168 | 24.057 | 32.987 | 57.390 | 1.00 | 33.29 | 6 |
| ATOM | 1328 | CG | ASP | A | 168 | 23.937 | 33.676 | 56.037 | 1.00 | 35.38 | 6 |
| ATOM | 1329 | OD1 | ASP | A | 168 | 24.892 | 34.388 | 55.659 | 1.00 | 39.48 | 8 |
| ATOM | 1330 | OD2 | ASP | A | 168 | 22.893 | 33.531 | 55.364 | 1.00 | 33.40 | 8 |
| ATOM | 1331 | C | ASP | A | 168 | 21.906 | 33.614 | 58.408 | 1.00 | 28.74 | 6 |
| ATOM | 1332 | O | ASP | A | 168 | 21.354 | 32.648 | 58.948 | 1.00 | 26.21 | 8 |
| ATOM | 1333 | N | ALA | A | 169 | 21.239 | 34.524 | 57.711 | 1.00 | 26.16 | 7 |
| ATOM | 1334 | CA | ALA | A | 169 | 19.793 | 34.415 | 57.579 | 1.00 | 24.39 | 6 |
| ATOM | 1335 | CB | ALA | A | 169 | 19.233 | 35.640 | 56.879 | 1.00 | 22.75 | 6 |
| ATOM | 1336 | C | ALA | A | 169 | 19.420 | 33.157 | 56.813 | 1.00 | 24.37 | 6 |
| ATOM | 1337 | O | ALA | A | 169 | 18.266 | 32.752 | 56.824 | 1.00 | 22.34 | 8 |
| ATOM | 1338 | N | HIS | A | 170 | 20.405 | 32.542 | 56.156 | 1.00 | 25.78 | 7 |
| ATOM | 1339 | CA | HIS | A | 170 | 20.180 | 31.327 | 55.375 | 1.00 | 25.20 | 6 |
| ATOM | 1340 | CB | HIS | A | 170 | 20.667 | 31.501 | 53.936 | 1.00 | 25.76 | 6 |
| ATOM | 1341 | CG | HIS | A | 170 | 20.122 | 32.711 | 53.245 | 1.00 | 29.08 | 6 |
| ATOM | 1342 | CD2 | HIS | A | 170 | 19.338 | 32.834 | 52.147 | 1.00 | 30.59 | 6 |
| ATOM | 1343 | ND1 | HIS | A | 170 | 20.384 | 33.995 | 53.675 | 1.00 | 30.77 | 7 |
| ATOM | 1344 | CE1 | HIS | A | 170 | 19.784 | 34.858 | 52.873 | 1.00 | 29.07 | 6 |
| ATOM | 1345 | NE2 | HIS | A | 170 | 19.143 | 34.180 | 51.939 | 1.00 | 32.19 | 7 |
| ATOM | 1346 | C | HIS | A | 170 | 20.895 | 30.113 | 55.958 | 1.00 | 26.00 | 6 |
| ATOM | 1347 | O | HIS | A | 170 | 21.913 | 30.234 | 56.637 | 1.00 | 25.76 | 8 |
| ATOM | 1348 | N | HIS | A | 171 | 20.349 | 28.939 | 55.658 | 1.00 | 27.29 | 7 |
| ATOM | 1349 | CA | HIS | A | 171 | 20.893 | 27.655 | 56.090 | 1.00 | 25.01 | 6 |
| ATOM | 1350 | CB | HIS | A | 171 | 19.934 | 26.532 | 55.663 | 1.00 | 24.93 | 6 |
| ATOM | 1351 | CG | HIS | A | 171 | 20.468 | 25.148 | 55.889 | 1.00 | 26.56 | 6 |
| ATOM | 1352 | CD2 | HIS | A | 171 | 20.674 | 24.123 | 55.028 | 1.00 | 22.34 | 6 |
| ATOM | 1353 | ND1 | HIS | A | 171 | 20.823 | 24.678 | 57.137 | 1.00 | 25.35 | 7 |
| ATOM | 1354 | CE1 | HIS | A | 171 | 21.222 | 23.424 | 57.036 | 1.00 | 22.68 | 6 |
| ATOM | 1355 | NE2 | HIS | A | 171 | 21.140 | 23.062 | 55.767 | 1.00 | 24.13 | 7 |
| ATOM | 1356 | C | HIS | A | 171 | 22.267 | 27.413 | 55.471 | 1.00 | 24.74 | 6 |
| ATOM | 1357 | O | HIS | A | 171 | 22.540 | 27.863 | 54.356 | 1.00 | 28.22 | 8 |
| ATOM | 1358 | N | CYS | A | 172 | 23.131 | 26.705 | 56.190 | 1.00 | 23.03 | 7 |
| ATOM | 1359 | CA | CYS | A | 172 | 24.467 | 26.389 | 55.683 | 1.00 | 23.41 | 6 |
| ATOM | 1360 | CB | CYS | A | 172 | 25.497 | 26.474 | 56.812 | 1.00 | 19.31 | 6 |
| ATOM | 1361 | SG | CYS | A | 172 | 25.005 | 25.631 | 58.318 | 1.00 | 16.78 | 16 |
| ATOM | 1362 | C | CYS | A | 172 | 24.484 | 24.997 | 55.048 | 1.00 | 25.45 | 6 |
| ATOM | 1363 | O | CYS | A | 172 | 25.203 | 24.098 | 55.483 | 1.00 | 24.47 | 8 |
| ATOM | 1364 | N | ASP | A | 173 | 23.664 | 24.839 | 54.015 | 1.00 | 26.67 | 7 |
| ATOM | 1365 | CA | ASP | A | 173 | 23.542 | 23.593 | 53.269 | 1.00 | 26.47 | 6 |
| ATOM | 1366 | CB | ASP | A | 173 | 22.735 | 23.857 | 51.993 | 1.00 | 26.33 | 6 |
| ATOM | 1367 | CG | ASP | A | 173 | 23.281 | 25.030 | 51.179 | 1.00 | 27.06 | 6 |
| ATOM | 1368 | OD1 | ASP | A | 173 | 22.539 | 25.558 | 50.330 | 1.00 | 23.43 | 8 |
| ATOM | 1369 | OD2 | ASP | A | 173 | 24.454 | 25.417 | 51.372 | 1.00 | 29.38 | 8 |
| ATOM | 1370 | C | ASP | A | 173 | 24.872 | 22.932 | 52.922 | 1.00 | 26.65 | 6 |
| ATOM | 1371 | O | ASP | A | 173 | 24.940 | 21.708 | 52.784 | 1.00 | 28.38 | 8 |
| ATOM | 1372 | N | GLY | A | 174 | 25.926 | 23.737 | 52.793 | 1.00 | 25.24 | 7 |
| ATOM | 1373 | CA | GLY | A | 174 | 27.227 | 23.198 | 52.447 | 1.00 | 23.11 | 6 |
| ATOM | 1374 | C | GLY | A | 174 | 27.896 | 22.505 | 53.612 | 1.00 | 25.64 | 6 |
| ATOM | 1375 | O | GLY | A | 174 | 28.443 | 21.408 | 53.462 | 1.00 | 27.67 | 8 |
| ATOM | 1376 | N | VAL | A | 175 | 27.848 | 23.144 | 54.778 | 1.00 | 24.29 | 7 |
| ATOM | 1377 | CA | VAL | A | 175 | 28.459 | 22.602 | 55.989 | 1.00 | 22.20 | 6 |
| ATOM | 1378 | CB | VAL | A | 175 | 28.536 | 23.672 | 57.101 | 1.00 | 20.15 | 6 |
| ATOM | 1379 | CG1 | VAL | A | 175 | 29.449 | 23.192 | 58.218 | 1.00 | 20.11 | 6 |
| ATOM | 1380 | CG2 | VAL | A | 175 | 29.015 | 24.989 | 56.530 | 1.00 | 18.74 | 6 |
| ATOM | 1381 | C | VAL | A | 175 | 27.647 | 21.409 | 56.505 | 1.00 | 22.85 | 6 |
| ATOM | 1382 | O | VAL | A | 175 | 28.173 | 20.512 | 57.173 | 1.00 | 20.07 | 8 |
| ATOM | 1383 | N | GLN | A | 176 | 26.356 | 21.404 | 56.203 | 1.00 | 24.12 | 7 |
| ATOM | 1384 | CA | GLN | A | 176 | 25.518 | 20.303 | 56.629 | 1.00 | 27.18 | 6 |
| ATOM | 1385 | CB | GLN | A | 176 | 24.045 | 20.611 | 56.355 | 1.00 | 32.86 | 6 |
| ATOM | 1386 | CG | GLN | A | 176 | 23.084 | 19.483 | 56.726 | 1.00 | 36.04 | 6 |

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Figure 17-22

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1387 | CD | GLN | A | 176 | 21.620 | 19.862 | 56.537 | 1.00 | 38.36 | 6 |
| ATOM | 1388 | OE1 | GLN | A | 176 | 21.113 | 20.782 | 57.185 | 1.00 | 38.59 | 8 |
| ATOM | 1389 | NE2 | GLN | A | 176 | 20.934 | 19.151 | 55.649 | 1.00 | 38.81 | 7 |
| ATOM | 1390 | C | GLN | A | 176 | 25.956 | 19.083 | 55.841 | 1.00 | 27.70 | 6 |
| ATOM | 1391 | O | GLN | A | 176 | 26.326 | 18.066 | 56.416 | 1.00 | 26.89 | 8 |
| ATOM | 1392 | N | GLU | A | 177 | 25.951 | 19.194 | 54.519 | 1.00 | 27.96 | 7 |
| ATOM | 1393 | CA | GLU | A | 177 | 26.343 | 18.062 | 53.698 | 1.00 | 31.16 | 6 |
| ATOM | 1394 | CB | GLU | A | 177 | 26.395 | 18.460 | 52.220 | 1.00 | 30.37 | 6 |
| ATOM | 1395 | CG | GLU | A | 177 | 26.353 | 17.256 | 51.287 | 1.00 | 36.20 | 6 |
| ATOM | 1396 | CD | GLU | A | 177 | 26.273 | 17.626 | 49.818 | 1.00 | 40.70 | 6 |
| ATOM | 1397 | OE1 | GLU | A | 177 | 27.322 | 17.967 | 49.234 | 1.00 | 46.78 | 8 |
| ATOM | 1398 | OE2 | GLU | A | 177 | 25.155 | 17.590 | 49.250 | 1.00 | 39.39 | 8 |
| ATOM | 1399 | C | GLU | A | 177 | 27.702 | 17.516 | 54.137 | 1.00 | 31.66 | 6 |
| ATOM | 1400 | O | GLU | A | 177 | 27.868 | 16.317 | 54.356 | 1.00 | 32.81 | 8 |
| ATOM | 1401 | N | ALA | A | 178 | 28.663 | 18.419 | 54.287 | 1.00 | 33.39 | 7 |
| ATOM | 1402 | CA | ALA | A | 178 | 30.026 | 18.072 | 54.673 | 1.00 | 31.63 | 6 |
| ATOM | 1403 | CB | ALA | A | 178 | 30.830 | 19.338 | 54.856 | 1.00 | 30.96 | 6 |
| ATOM | 1404 | C | ALA | A | 178 | 30.204 | 17.185 | 55.897 | 1.00 | 30.63 | 6 |
| ATOM | 1405 | O | ALA | A | 178 | 31.032 | 16.276 | 55.876 | 1.00 | 27.95 | 8 |
| ATOM | 1406 | N | PHE | A | 179 | 29.444 | 17.444 | 56.961 | 1.00 | 31.01 | 7 |
| ATOM | 1407 | CA | PHE | A | 179 | 29.590 | 16.656 | 58.184 | 1.00 | 31.34 | 6 |
| ATOM | 1408 | CB | PHE | A | 179 | 30.147 | 17.532 | 59.310 | 1.00 | 30.13 | 6 |
| ATOM | 1409 | CG | PHE | A | 179 | 31.189 | 18.505 | 58.858 | 1.00 | 27.78 | 6 |
| ATOM | 1410 | CD1 | PHE | A | 179 | 30.827 | 19.790 | 58.466 | 1.00 | 28.24 | 6 |
| ATOM | 1411 | CD2 | PHE | A | 179 | 32.522 | 18.124 | 58.766 | 1.00 | 28.33 | 6 |
| ATOM | 1412 | CE1 | PHE | A | 179 | 31.778 | 20.688 | 57.988 | 1.00 | 26.68 | 6 |
| ATOM | 1413 | CE2 | PHE | A | 179 | 33.487 | 19.013 | 58.285 | 1.00 | 28.79 | 6 |
| ATOM | 1414 | CZ | PHE | A | 179 | 33.111 | 20.300 | 57.895 | 1.00 | 28.67 | 6 |
| ATOM | 1415 | C | PHE | A | 179 | 28.300 | 16.003 | 58.664 | 1.00 | 32.06 | 6 |
| ATOM | 1416 | O | PHE | A | 179 | 28.218 | 15.542 | 59.803 | 1.00 | 30.58 | 8 |
| ATOM | 1417 | N | TYR | A | 180 | 27.305 | 15.960 | 57.787 | 1.00 | 34.25 | 7 |
| ATOM | 1418 | CA | TYR | A | 180 | 26.001 | 15.377 | 58.099 | 1.00 | 38.60 | 6 |
| ATOM | 1419 | CB | TYR | A | 180 | 25.062 | 15.605 | 56.911 | 1.00 | 38.99 | 6 |
| ATOM | 1420 | CG | TYR | A | 180 | 23.593 | 15.453 | 57.220 | 1.00 | 37.91 | 6 |
| ATOM | 1421 | CD1 | TYR | A | 180 | 22.938 | 14.232 | 57.064 | 1.00 | 35.83 | 6 |
| ATOM | 1422 | CE1 | TYR | A | 180 | 21.589 | 14.103 | 57.373 | 1.00 | 39.20 | 6 |
| ATOM | 1423 | CD2 | TYR | A | 180 | 22.861 | 16.543 | 57.694 | 1.00 | 37.56 | 6 |
| ATOM | 1424 | CE2 | TYR | A | 180 | 21.518 | 16.430 | 58.007 | 1.00 | 40.28 | 6 |
| ATOM | 1425 | CZ | TYR | A | 180 | 20.882 | 15.211 | 57.848 | 1.00 | 41.92 | 6 |
| ATOM | 1426 | OH | TYR | A | 180 | 19.549 | 15.110 | 58.188 | 1.00 | 43.41 | 8 |
| ATOM | 1427 | C | TYR | A | 180 | 26.133 | 13.884 | 58.382 | 1.00 | 40.28 | 6 |
| ATOM | 1428 | O | TYR | A | 180 | 25.158 | 13.192 | 58.680 | 1.00 | 39.27 | 8 |
| ATOM | 1429 | N | ASP | A | 181 | 27.363 | 13.402 | 58.319 | 1.00 | 43.51 | 7 |
| ATOM | 1430 | CA | ASP | A | 181 | 27.638 | 11.994 | 58.519 | 1.00 | 45.89 | 6 |
| ATOM | 1431 | CB | ASP | A | 181 | 28.414 | 11.487 | 57.303 | 1.00 | 51.00 | 6 |
| ATOM | 1432 | CG | ASP | A | 181 | 28.830 | 10.050 | 57.436 | 1.00 | 56.84 | 6 |
| ATOM | 1433 | OD1 | ASP | A | 181 | 29.637 | 9.750 | 58.345 | 1.00 | 59.47 | 8 |
| ATOM | 1434 | OD2 | ASP | A | 181 | 28.348 | 9.221 | 56.629 | 1.00 | 60.73 | 8 |
| ATOM | 1435 | C | ASP | A | 181 | 28.398 | 11.665 | 59.804 | 1.00 | 44.75 | 6 |
| ATOM | 1436 | O | ASP | A | 181 | 28.257 | 10.568 | 60.350 | 1.00 | 44.69 | 8 |
| ATOM | 1437 | N | THR | A | 182 | 29.194 | 12.506 | 60.298 | 1.00 | 41.26 | 7 |
| ATOM | 1438 | CA | THR | A | 182 | 29.975 | 12.337 | 61.495 | 1.00 | 39.51 | 6 |
| ATOM | 1439 | CB | THR | A | 182 | 31.408 | 12.881 | 61.355 | 1.00 | 39.19 | 6 |
| ATOM | 1440 | OG1 | THR | A | 182 | 32.171 | 12.508 | 62.505 | 1.00 | 37.82 | 8 |
| ATOM | 1441 | CG2 | THR | A | 182 | 31.395 | 14.397 | 61.232 | 1.00 | 40.12 | 6 |
| ATOM | 1442 | C | THR | A | 182 | 29.370 | 12.910 | 62.759 | 1.00 | 38.58 | 6 |
| ATOM | 1443 | O | THR | A | 182 | 28.609 | 13.876 | 62.716 | 1.00 | 41.24 | 8 |
| ATOM | 1444 | N | ASP | A | 183 | 29.712 | 12.304 | 63.890 | 1.00 | 37.39 | 7 |
| ATOM | 1445 | CA | ASP | A | 183 | 29.211 | 12.773 | 65.171 | 1.00 | 39.24 | 6 |
| ATOM | 1446 | CB | ASP | A | 183 | 28.824 | 11.588 | 66.061 | 1.00 | 40.31 | 6 |
| ATOM | 1447 | CG | ASP | A | 183 | 30.010 | 10.723 | 66.433 | 1.00 | 41.64 | 6 |
| ATOM | 1448 | OD1 | ASP | A | 183 | 30.725 | 10.268 | 65.520 | 1.00 | 42.53 | 8 |
| ATOM | 1449 | OD2 | ASP | A | 183 | 30.221 | 10.494 | 67.640 | 1.00 | 42.46 | 8 |
| ATOM | 1450 | C | ASP | A | 183 | 30.286 | 13.621 | 65.853 | 1.00 | 40.34 | 6 |
| ATOM | 1451 | O | ASP | A | 183 | 30.109 | 14.071 | 66.983 | 1.00 | 42.07 | 8 |
| ATOM | 1452 | N | GLN | A | 184 | 31.400 | 13.830 | 65.154 | 1.00 | 39.29 | 7 |

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Figure 17-23

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1453 | CA | GLN | A | 184 | 32.506 | 14.635 | 65.671 | 1.00 | 37.08 | 6 |
| ATOM | 1454 | CB | GLN | A | 184 | 33.830 | 14.252 | 64.994 | 1.00 | 33.77 | 6 |
| ATOM | 1455 | CG | GLN | A | 184 | 34.229 | 12.804 | 65.166 | 1.00 | 33.63 | 6 |
| ATOM | 1456 | CD | GLN | A | 184 | 35.599 | 12.499 | 64.593 | 1.00 | 32.74 | 6 |
| ATOM | 1457 | OE1 | GLN | A | 184 | 35.853 | 12.704 | 63.413 | 1.00 | 31.17 | 8 |
| ATOM | 1458 | NE2 | GLN | A | 184 | 36.490 | 11.999 | 65.436 | 1.00 | 36.58 | 7 |
| ATOM | 1459 | C | GLN | A | 184 | 32.222 | 16.110 | 65.403 | 1.00 | 36.42 | 6 |
| ATOM | 1460 | O | GLN | A | 184 | 32.803 | 16.994 | 66.034 | 1.00 | 37.41 | 8 |
| ATOM | 1461 | N | VAL | A | 185 | 31.329 | 16.372 | 64.456 | 1.00 | 33.14 | 7 |
| ATOM | 1462 | CA | VAL | A | 185 | 30.984 | 17.740 | 64.119 | 1.00 | 32.40 | 6 |
| ATOM | 1463 | CB | VAL | A | 185 | 31.308 | 18.052 | 62.641 | 1.00 | 33.03 | 6 |
| ATOM | 1464 | CG1 | VAL | A | 185 | 31.009 | 19.520 | 62.331 | 1.00 | 29.27 | 6 |
| ATOM | 1465 | CG2 | VAL | A | 185 | 32.773 | 17.738 | 62.357 | 1.00 | 34.58 | 6 |
| ATOM | 1466 | C | VAL | A | 185 | 29.508 | 17.972 | 64.360 | 1.00 | 31.51 | 6 |
| ATOM | 1467 | O | VAL | A | 185 | 28.680 | 17.124 | 64.038 | 1.00 | 31.71 | 8 |
| ATOM | 1468 | N | PHE | A | 186 | 29.185 | 19.119 | 64.946 | 1.00 | 30.98 | 7 |
| ATOM | 1469 | CA | PHE | A | 186 | 27.798 | 19.463 | 65.207 | 1.00 | 31.44 | 6 |
| ATOM | 1470 | CB | PHE | A | 186 | 27.524 | 19.532 | 66.716 | 1.00 | 30.96 | 6 |
| ATOM | 1471 | CG | PHE | A | 186 | 26.059 | 19.617 | 67.066 | 1.00 | 31.59 | 6 |
| ATOM | 1472 | CD1 | PHE | A | 186 | 25.552 | 18.901 | 68.153 | 1.00 | 30.54 | 6 |
| ATOM | 1473 | CD2 | PHE | A | 186 | 25.179 | 20.395 | 66.308 | 1.00 | 31.50 | 6 |
| ATOM | 1474 | CE1 | PHE | A | 186 | 24.191 | 18.951 | 68.478 | 1.00 | 33.28 | 6 |
| ATOM | 1475 | CE2 | PHE | A | 186 | 23.815 | 20.457 | 66.622 | 1.00 | 33.04 | 6 |
| ATOM | 1476 | CZ | PHE | A | 186 | 23.318 | 19.733 | 67.708 | 1.00 | 32.35 | 6 |
| ATOM | 1477 | C | PHE | A | 186 | 27.490 | 20.798 | 64.551 | 1.00 | 30.37 | 6 |
| ATOM | 1478 | O | PHE | A | 186 | 28.189 | 21.789 | 64.751 | 1.00 | 31.32 | 8 |
| ATOM | 1479 | N | VAL | A | 187 | 26.435 | 20.809 | 63.752 | 1.00 | 31.14 | 7 |
| ATOM | 1480 | CA | VAL | A | 187 | 26.024 | 22.015 | 63.063 | 1.00 | 32.05 | 6 |
| ATOM | 1481 | CB | VAL | A | 187 | 26.018 | 21.805 | 61.525 | 1.00 | 33.54 | 6 |
| ATOM | 1482 | CG1 | VAL | A | 187 | 25.574 | 23.081 | 60.813 | 1.00 | 32.07 | 6 |
| ATOM | 1483 | CG2 | VAL | A | 187 | 27.420 | 21.389 | 61.056 | 1.00 | 35.44 | 6 |
| ATOM | 1484 | C | VAL | A | 187 | 24.638 | 22.439 | 63.524 | 1.00 | 31.47 | 6 |
| ATOM | 1485 | O | VAL | A | 187 | 23.666 | 21.686 | 63.410 | 1.00 | 29.06 | 8 |
| ATOM | 1486 | N | LEU | A | 188 | 24.579 | 23.638 | 64.090 | 1.00 | 29.44 | 7 |
| ATOM | 1487 | CA | LEU | A | 188 | 23.336 | 24.228 | 64.551 | 1.00 | 29.39 | 6 |
| ATOM | 1488 | CB | LEU | A | 188 | 23.433 | 24.665 | 66.009 | 1.00 | 29.62 | 6 |
| ATOM | 1489 | CG | LEU | A | 188 | 22.293 | 25.589 | 66.458 | 1.00 | 27.92 | 5 |
| ATOM | 1490 | CD1 | LEU | A | 188 | 20.970 | 24.844 | 66.414 | 1.00 | 25.87 | 6 |
| ATOM | 1491 | CD2 | LEU | A | 188 | 22.574 | 26.107 | 67.861 | 1.00 | 27.69 | 6 |
| ATOM | 1492 | C | LEU | A | 188 | 23.161 | 25.454 | 63.675 | 1.00 | 31.89 | 6 |
| ATOM | 1493 | O | LEU | A | 188 | 24.130 | 26.175 | 63.388 | 1.00 | 31.50 | 8 |
| ATOM | 1494 | N | SER | A | 189 | 21.929 | 25.700 | 63.250 | 1.00 | 29.93 | 7 |
| ATOM | 1495 | CA | SER | A | 189 | 21.682 | 26.831 | 62.390 | 1.00 | 24.65 | 6 |
| ATOM | 1496 | CB | SER | A | 189 | 21.873 | 26.411 | 60.942 | 1.00 | 22.40 | 6 |
| ATOM | 1497 | OG | SER | A | 189 | 21.585 | 27.485 | 60.083 | 1.00 | 19.12 | 8 |
| ATOM | 1498 | C | SER | A | 189 | 20.716 | 27.462 | 62.540 | 1.00 | 27.00 | 6 |
| ATOM | 1499 | O | SER | A | 189 | 19.296 | 26.774 | 62.577 | 1.00 | 26.72 | 8 |
| ATOM | 1500 | N | LEU | A | 190 | 20.521 | 28.783 | 62.669 | 1.00 | 27.41 | 7 |
| ATOM | 1501 | CA | LEU | A | 190 | 19.096 | 29.554 | 62.735 | 1.00 | 29.68 | 6 |
| ATOM | 1502 | CB | LEU | A | 190 | 19.185 | 30.682 | 63.771 | 1.00 | 29.84 | 6 |
| ATOM | 1503 | CG | LEU | A | 190 | 19.108 | 30.366 | 65.264 | 1.00 | 26.79 | 6 |
| ATOM | 1504 | CD1 | LEU | A | 190 | 19.020 | 31.662 | 66.045 | 1.00 | 23.44 | 6 |
| ATOM | 1505 | CD2 | LEU | A | 190 | 17.881 | 29.549 | 65.546 | 1.00 | 27.63 | 6 |
| ATOM | 1506 | C | LEU | A | 190 | 19.046 | 30.141 | 61.329 | 1.00 | 29.58 | 6 |
| ATOM | 1507 | O | LEU | A | 190 | 20.084 | 30.525 | 60.790 | 1.00 | 32.40 | 8 |
| ATOM | 1508 | N | HIS | A | 191 | 17.864 | 30.206 | 60.727 | 1.00 | 29.61 | 7 |
| ATOM | 1509 | CA | HIS | A | 191 | 17.766 | 30.726 | 59.368 | 1.00 | 29.72 | 6 |
| ATOM | 1510 | CB | HIS | A | 191 | 18.595 | 29.839 | 58.432 | 1.00 | 26.47 | 6 |
| ATOM | 1511 | CG | HIS | A | 191 | 18.225 | 28.392 | 58.504 | 1.00 | 28.18 | 6 |
| ATOM | 1512 | CD2 | HIS | A | 191 | 18.918 | 27.313 | 58.940 | 1.00 | 28.88 | 6 |
| ATOM | 1513 | ND1 | HIS | A | 191 | 16.989 | 27.921 | 58.118 | 1.00 | 31.00 | 7 |
| ATOM | 1514 | CE1 | HIS | A | 191 | 16.938 | 26.614 | 58.312 | 1.00 | 30.54 | 6 |
| ATOM | 1515 | NE2 | HIS | A | 191 | 18.095 | 26.220 | 58.810 | 1.00 | 27.21 | 7 |
| ATOM | 1516 | C | HIS | A | 191 | 16.329 | 30.812 | 58.856 | 1.00 | 28.05 | 6 |
| ATOM | 1517 | O | HIS | A | 191 | 15.385 | 30.411 | 59.535 | 1.00 | 27.81 | 8 |
| ATOM | 1518 | N | GLN | A | 192 | 16.183 | 31.346 | 57.649 | 1.00 | 29.39 | 7 |

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Figure 17-24

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1519 | CA | GLN | A | 192 | 14.886 | 31.494 | 57.008 | 1.00 | 28.21 | 6 |
| ATOM | 1520 | CB | GLN | A | 192 | 15.016 | 32.416 | 55.796 | 1.00 | 24.94 | 6 |
| ATOM | 1521 | CG | GLN | A | 192 | 15.622 | 33.773 | 56.124 | 1.00 | 21.66 | 6 |
| ATOM | 1522 | CD | GLN | A | 192 | 15.701 | 34.690 | 54.921 | 1.00 | 22.22 | 6 |
| ATOM | 1523 | OE1 | GLN | A | 192 | 14.684 | 35.173 | 54.428 | 1.00 | 23.38 | 8 |
| ATOM | 1524 | NE2 | GLN | A | 192 | 16.914 | 34.925 | 54.434 | 1.00 | 22.97 | 7 |
| ATOM | 1525 | C | GLN | A | 192 | 14.435 | 30.104 | 56.570 | 1.00 | 32.71 | 6 |
| ATOM | 1526 | O | GLN | A | 192 | 15.157 | 29.403 | 55.853 | 1.00 | 33.85 | 8 |
| ATOM | 1527 | N | SER | A | 193 | 13.249 | 29.694 | 57.011 | 1.00 | 34.44 | 7 |
| ATOM | 1528 | CA | SER | A | 193 | 12.751 | 28.376 | 56.650 | 1.00 | 33.28 | 6 |
| ATOM | 1529 | CB | SER | A | 193 | 11.264 | 28.249 | 56.961 | 1.00 | 33.25 | 6 |
| ATOM | 1530 | OG | SER | A | 193 | 10.786 | 26.987 | 56.540 | 1.00 | 31.52 | 8 |
| ATOM | 1531 | C | SER | A | 193 | 12.974 | 28.150 | 55.171 | 1.00 | 34.79 | 6 |
| ATOM | 1532 | O | SER | A | 193 | 12.775 | 29.051 | 54.356 | 1.00 | 33.74 | 8 |
| ATOM | 1533 | N | PRO | A | 194 | 13.404 | 26.938 | 54.803 | 1.00 | 37.57 | 7 |
| ATOM | 1534 | CD | PRO | A | 194 | 13.689 | 25.775 | 55.658 | 1.00 | 38.89 | 6 |
| ATOM | 1535 | CA | PRO | A | 194 | 13.654 | 26.600 | 53.403 | 1.00 | 37.81 | 6 |
| ATOM | 1536 | CB | PRO | A | 194 | 14.248 | 25.194 | 53.498 | 1.00 | 39.30 | 6 |
| ATOM | 1537 | CG | PRO | A | 194 | 14.840 | 25.163 | 54.916 | 1.00 | 39.09 | 6 |
| ATOM | 1538 | C | PRO | A | 194 | 12.340 | 26.617 | 52.638 | 1.00 | 36.81 | 6 |
| ATOM | 1539 | O | PRO | A | 194 | 12.317 | 26.443 | 51.425 | 1.00 | 34.09 | 8 |
| ATOM | 1540 | N | GLU | A | 195 | 11.246 | 26.835 | 53.364 | 1.00 | 39.25 | 7 |
| ATOM | 1541 | CA | GLU | A | 195 | 9.928 | 26.866 | 52.750 | 1.00 | 41.54 | 6 |
| ATOM | 1542 | CB | GLU | A | 195 | 8.843 | 26.600 | 53.812 | 1.00 | 45.84 | 6 |
| ATOM | 1543 | CG | GLU | A | 195 | 8.360 | 27.811 | 54.608 | 1.00 | 53.30 | 6 |
| ATOM | 1544 | CD | GLU | A | 195 | 7.160 | 28.502 | 53.960 | 1.00 | 55.91 | 6 |
| ATOM | 1545 | OE1 | GLU | A | 195 | 6.735 | 29.571 | 54.461 | 1.00 | 55.14 | 8 |
| ATOM | 1546 | OE2 | GLU | A | 195 | 6.631 | 27.966 | 52.956 | 1.00 | 57.75 | 8 |
| ATOM | 1547 | C | GLU | A | 195 | 9.700 | 28.208 | 52.047 | 1.00 | 39.50 | 6 |
| ATOM | 1548 | O | GLU | A | 195 | 8.651 | 28.431 | 51.452 | 1.00 | 40.21 | 8 |
| ATOM | 1549 | N | TYR | A | 196 | 10.689 | 29.096 | 52.098 | 1.00 | 37.13 | 7 |
| ATOM | 1550 | CA | TYR | A | 196 | 10.549 | 30.379 | 51.434 | 1.00 | 35.50 | 6 |
| ATOM | 1551 | CB | TYR | A | 196 | 9.602 | 31.274 | 52.245 | 1.00 | 36.36 | 6 |
| ATOM | 1552 | CG | TYR | A | 196 | 10.175 | 31.816 | 53.538 | 1.00 | 37.28 | 6 |
| ATOM | 1553 | CD1 | TYR | A | 196 | 11.120 | 32.848 | 53.527 | 1.00 | 35.42 | 6 |
| ATOM | 1554 | CE1 | TYR | A | 196 | 11.637 | 33.366 | 54.706 | 1.00 | 33.10 | 6 |
| ATOM | 1555 | CD2 | TYR | A | 196 | 9.764 | 31.311 | 54.776 | 1.00 | 36.75 | 6 |
| ATOM | 1556 | CE2 | TYR | A | 196 | 10.279 | 31.825 | 55.968 | 1.00 | 35.26 | 6 |
| ATOM | 1557 | CZ | TYR | A | 196 | 11.213 | 32.856 | 55.922 | 1.00 | 35.84 | 6 |
| ATOM | 1558 | OH | TYR | A | 196 | 11.704 | 33.401 | 57.087 | 1.00 | 37.09 | 8 |
| ATOM | 1559 | C | TYR | A | 196 | 11.878 | 31.097 | 51.188 | 1.00 | 34.89 | 6 |
| ATOM | 1560 | O | TYR | A | 196 | 11.896 | 32.256 | 50.764 | 1.00 | 31.61 | 8 |
| ATOM | 1561 | N | ALA | A | 197 | 12.991 | 30.416 | 51.437 | 1.00 | 34.39 | 7 |
| ATOM | 1562 | CA | ALA | A | 197 | 14.297 | 31.041 | 51.242 | 1.00 | 34.82 | 6 |
| ATOM | 1563 | CB | ALA | A | 197 | 14.684 | 31.826 | 52.489 | 1.00 | 32.48 | 6 |
| ATOM | 1564 | C | ALA | A | 197 | 15.418 | 30.075 | 50.887 | 1.00 | 36.59 | 6 |
| ATOM | 1565 | O | ALA | A | 197 | 15.407 | 28.903 | 51.291 | 1.00 | 37.46 | 8 |
| ATOM | 1566 | N | PHE | A | 198 | 16.388 | 30.584 | 50.133 | 1.00 | 36.22 | 7 |
| ATOM | 1567 | CA | PHE | A | 198 | 17.548 | 29.802 | 49.722 | 1.00 | 37.68 | 6 |
| ATOM | 1568 | CB | PHE | A | 198 | 18.597 | 30.729 | 49.109 | 1.00 | 40.89 | 6 |
| ATOM | 1569 | CG | PHE | A | 198 | 19.810 | 30.013 | 48.578 | 1.00 | 43.59 | 6 |
| ATOM | 1570 | CD1 | PHE | A | 198 | 19.783 | 29.404 | 47.325 | 1.00 | 44.74 | 6 |
| ATOM | 1571 | CD2 | PHE | A | 198 | 20.970 | 29.929 | 49.336 | 1.00 | 41.86 | 6 |
| ATOM | 1572 | CE1 | PHE | A | 198 | 20.894 | 28.729 | 46.833 | 1.00 | 41.42 | 6 |
| ATOM | 1573 | CE2 | PHE | A | 198 | 22.079 | 29.251 | 48.849 | 1.00 | 43.30 | 6 |
| ATOM | 1574 | CZ | PHE | A | 198 | 22.040 | 28.652 | 47.595 | 1.00 | 41.86 | 6 |
| ATOM | 1575 | C | PHE | A | 198 | 18.139 | 29.140 | 50.967 | 1.00 | 37.00 | 6 |
| ATOM | 1576 | O | PHE | A | 198 | 18.166 | 29.754 | 52.036 | 1.00 | 36.43 | 8 |
| ATOM | 1577 | N | PRO | A | 199 | 18.641 | 27.892 | 50.848 | 1.00 | 37.63 | 7 |
| ATOM | 1578 | CD | PRO | A | 199 | 19.298 | 27.238 | 51.997 | 1.00 | 35.29 | 6 |
| ATOM | 1579 | CA | PRO | A | 199 | 18.727 | 27.008 | 49.673 | 1.00 | 36.52 | 6 |
| ATOM | 1580 | CB | PRO | A | 199 | 19.702 | 25.936 | 50.138 | 1.00 | 34.96 | 6 |
| ATOM | 1581 | CG | PRO | A | 199 | 19.281 | 25.770 | 51.565 | 1.00 | 34.57 | 6 |
| ATOM | 1582 | C | PRO | A | 199 | 17.409 | 26.380 | 49.222 | 1.00 | 35.72 | 6 |
| ATOM | 1583 | O | PRO | A | 199 | 17.386 | 25.663 | 48.225 | 1.00 | 37.36 | 8 |
| ATOM | 1584 | N | PHE | A | 200 | 16.331 | 26.638 | 49.962 | 1.00 | 33.78 | 7 |

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Figure 17-25

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1585 | CA | PHE | A | 200 | 15.004 | 26.090 | 49.662 | 1.00 | 32.15 | 6 |
| ATOM | 1586 | CB | PHE | A | 200 | 14.562 | 26.381 | 48.222 | 1.00 | 28.39 | 6 |
| ATOM | 1587 | CG | PHE | A | 200 | 14.600 | 27.827 | 47.835 | 1.00 | 26.29 | 6 |
| ATOM | 1588 | CD1 | PHE | A | 200 | 15.749 | 28.385 | 47.296 | 1.00 | 24.82 | 6 |
| ATOM | 1589 | CD2 | PHE | A | 200 | 13.466 | 28.623 | 47.966 | 1.00 | 28.04 | 6 |
| ATOM | 1590 | CE1 | PHE | A | 200 | 15.767 | 29.712 | 46.882 | 1.00 | 25.68 | 6 |
| ATOM | 1591 | CE2 | PHE | A | 200 | 13.475 | 29.955 | 47.557 | 1.00 | 27.03 | 6 |
| ATOM | 1592 | CZ | PHE | A | 200 | 14.626 | 30.498 | 47.013 | 1.00 | 24.90 | 6 |
| ATOM | 1593 | C | PHE | A | 200 | 14.947 | 24.574 | 49.842 | 1.00 | 32.66 | 6 |
| ATOM | 1594 | O | PHE | A | 200 | 13.925 | 24.033 | 50.264 | 1.00 | 31.22 | 8 |
| ATOM | 1595 | N | GLU | A | 201 | 16.043 | 23.896 | 49.499 | 1.00 | 33.60 | 7 |
| ATOM | 1596 | CA | GLU | A | 201 | 16.128 | 22.438 | 49.585 | 1.00 | 30.86 | 6 |
| ATOM | 1597 | CB | GLU | A | 201 | 17.213 | 21.931 | 48.637 | 1.00 | 32.98 | 6 |
| ATOM | 1598 | CG | GLU | A | 201 | 16.879 | 22.182 | 47.175 | 1.00 | 33.52 | 6 |
| ATOM | 1599 | CD | GLU | A | 201 | 18.012 | 21.864 | 46.232 | 1.00 | 34.56 | 6 |
| ATOM | 1600 | OE1 | GLU | A | 201 | 18.396 | 20.678 | 46.117 | 1.00 | 36.35 | 8 |
| ATOM | 1601 | OE2 | GLU | A | 201 | 18.523 | 22.814 | 45.605 | 1.00 | 36.52 | 8 |
| ATOM | 1602 | C | GLU | A | 201 | 16.369 | 21.911 | 50.981 | 1.00 | 28.52 | 6 |
| ATOM | 1603 | O | GLU | A | 201 | 15.537 | 21.199 | 51.520 | 1.00 | 28.91 | 8 |
| ATOM | 1604 | N | LYS | A | 202 | 17.511 | 22.239 | 51.566 | 1.00 | 31.64 | 7 |
| ATOM | 1605 | CA | LYS | A | 202 | 17.795 | 21.780 | 52.917 | 1.00 | 32.34 | 6 |
| ATOM | 1606 | CB | LYS | A | 202 | 19.276 | 21.432 | 53.092 | 1.00 | 36.91 | 6 |
| ATOM | 1607 | CG | LYS | A | 202 | 19.789 | 20.226 | 52.307 | 1.00 | 43.74 | 6 |
| ATOM | 1608 | CD | LYS | A | 202 | 20.212 | 20.590 | 50.891 | 1.00 | 49.31 | 6 |
| ATOM | 1609 | CE | LYS | A | 202 | 20.952 | 19.428 | 50.227 | 1.00 | 49.34 | 6 |
| ATOM | 1610 | NZ | LYS | A | 202 | 21.504 | 19.802 | 48.895 | 1.00 | 49.89 | 7 |
| ATOM | 1611 | C | LYS | A | 202 | 17.421 | 22.849 | 53.937 | 1.00 | 30.55 | 6 |
| ATOM | 1612 | O | LYS | A | 202 | 16.877 | 23.890 | 53.586 | 1.00 | 26.55 | 8 |
| ATOM | 1613 | N | GLY | A | 203 | 17.710 | 22.571 | 55.203 | 1.00 | 30.59 | 7 |
| ATOM | 1614 | CA | GLY | A | 203 | 17.422 | 23.519 | 56.259 | 1.00 | 30.24 | 6 |
| ATOM | 1615 | C | GLY | A | 203 | 16.216 | 23.210 | 57.125 | 1.00 | 29.23 | 6 |
| ATOM | 1616 | O | GLY | A | 203 | 15.915 | 23.975 | 58.041 | 1.00 | 32.90 | 8 |
| ATOM | 1617 | N | PHE | A | 204 | 15.526 | 22.104 | 56.866 | 1.00 | 26.32 | 7 |
| ATOM | 1618 | CA | PHE | A | 204 | 14.344 | 21.779 | 57.657 | 1.00 | 23.25 | 6 |
| ATOM | 1619 | CB | PHE | A | 204 | 13.366 | 20.917 | 56.863 | 1.00 | 21.25 | 6 |
| ATOM | 1620 | CG | PHE | A | 204 | 12.855 | 21.573 | 55.635 | 1.00 | 18.60 | 6 |
| ATOM | 1621 | CD1 | PHE | A | 204 | 13.605 | 21.560 | 54.461 | 1.00 | 16.43 | 6 |
| ATOM | 1622 | CD2 | PHE | A | 204 | 11.654 | 22.273 | 55.664 | 1.00 | 14.82 | 6 |
| ATOM | 1623 | CE1 | PHE | A | 204 | 13.168 | 22.245 | 53.333 | 1.00 | 16.91 | 6 |
| ATOM | 1624 | CE2 | PHE | A | 204 | 11.206 | 22.962 | 54.544 | 1.00 | 15.28 | 6 |
| ATOM | 1625 | CZ | PHE | A | 204 | 11.965 | 22.952 | 53.375 | 1.00 | 18.34 | 6 |
| ATOM | 1626 | C | PHE | A | 204 | 14.626 | 21.094 | 58.979 | 1.00 | 23.72 | 6 |
| ATOM | 1627 | O | PHE | A | 204 | 15.578 | 20.318 | 59.118 | 1.00 | 22.68 | 8 |
| ATOM | 1628 | N | LEU | A | 205 | 13.760 | 21.376 | 59.942 | 1.00 | 20.94 | 7 |
| ATOM | 1629 | CA | LEU | A | 205 | 13.877 | 20.818 | 61.272 | 1.00 | 24.83 | 6 |
| ATOM | 1630 | CB | LEU | A | 205 | 12.678 | 21.259 | 62.110 | 1.00 | 21.29 | 6 |
| ATOM | 1631 | CG | LEU | A | 205 | 12.672 | 20.811 | 63.568 | 1.00 | 22.67 | 6 |
| ATOM | 1632 | CD1 | LEU | A | 205 | 14.011 | 21.182 | 64.245 | 1.00 | 19.76 | 6 |
| ATOM | 1633 | CD2 | LEU | A | 205 | 11.478 | 21.456 | 64.275 | 1.00 | 20.62 | 6 |
| ATOM | 1634 | C | LEU | A | 205 | 14.002 | 19.293 | 61.303 | 1.00 | 28.79 | 6 |
| ATOM | 1635 | O | LEU | A | 205 | 14.443 | 18.730 | 62.310 | 1.00 | 28.59 | 8 |
| ATOM | 1636 | N | GLU | A | 206 | 13.625 | 18.628 | 60.211 | 1.00 | 33.52 | 7 |
| ATOM | 1637 | CA | GLU | A | 206 | 13.693 | 17.166 | 60.142 | 1.00 | 39.79 | 6 |
| ATOM | 1638 | CB | GLU | A | 206 | 12.736 | 16.616 | 59.070 | 1.00 | 44.37 | 6 |
| ATOM | 1639 | CG | GLU | A | 206 | 11.284 | 17.060 | 59.204 | 1.00 | 50.75 | 6 |
| ATOM | 1640 | CD | GLU | A | 206 | 11.014 | 18.390 | 58.512 | 1.00 | 55.31 | 6 |
| ATOM | 1641 | OE1 | GLU | A | 206 | 9.972 | 19.027 | 58.797 | 1.00 | 55.36 | 8 |
| ATOM | 1642 | OE2 | GLU | A | 206 | 11.839 | 18.786 | 57.661 | 1.00 | 56.48 | 8 |
| ATOM | 1643 | C | GLU | A | 206 | 15.114 | 16.674 | 59.847 | 1.00 | 40.00 | 6 |
| ATOM | 1644 | O | GLU | A | 206 | 15.483 | 15.541 | 60.180 | 1.00 | 39.35 | 8 |
| ATOM | 1645 | N | GLU | A | 207 | 15.903 | 17.536 | 59.217 | 1.00 | 39.38 | 7 |
| ATOM | 1646 | CA | GLU | A | 207 | 17.286 | 17.219 | 58.873 | 1.00 | 37.90 | 6 |
| ATOM | 1647 | CB | GLU | A | 207 | 17.776 | 18.242 | 57.854 | 1.00 | 37.36 | 6 |
| ATOM | 1648 | CG | GLU | A | 207 | 16.983 | 18.158 | 56.556 | 1.00 | 37.29 | 6 |
| ATOM | 1649 | CD | GLU | A | 207 | 16.978 | 19.452 | 55.773 | 1.00 | 38.16 | 6 |
| ATOM | 1650 | OE1 | GLU | A | 207 | 18.071 | 20.016 | 55.537 | 1.00 | 35.44 | 8 |

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Figure 17-26

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1651 | OE2 | GLU | A | 207 | 15.870 | 19.891 | 55.389 | 1.00 | 34.62 | 8 |
| ATOM | 1652 | C | GLU | A | 207 | 18.139 | 17.239 | 60.134 | 1.00 | 36.18 | 6 |
| ATOM | 1653 | O | GLU | A | 207 | 18.560 | 18.303 | 60.590 | 1.00 | 34.81 | 8 |
| ATOM | 1654 | N | ILE | A | 208 | 18.381 | 16.059 | 60.701 | 1.00 | 34.45 | 7 |
| ATOM | 1655 | CA | ILE | A | 208 | 19.164 | 15.965 | 61.932 | 1.00 | 38.53 | 6 |
| ATOM | 1656 | CB | ILE | A | 208 | 18.260 | 15.511 | 63.117 | 1.00 | 41.12 | 6 |
| ATOM | 1657 | CG2 | ILE | A | 208 | 19.097 | 15.273 | 64.375 | 1.00 | 41.36 | 6 |
| ATOM | 1658 | CG1 | ILE | A | 208 | 17.193 | 16.581 | 63.383 | 1.00 | 42.21 | 6 |
| ATOM | 1659 | CD1 | ILE | A | 208 | 16.291 | 16.286 | 64.560 | 1.00 | 44.81 | 6 |
| ATOM | 1660 | C | ILE | A | 208 | 20.407 | 15.074 | 61.876 | 1.00 | 36.66 | 6 |
| ATOM | 1661 | O | ILE | A | 208 | 21.243 | 15.110 | 62.775 | 1.00 | 34.03 | 8 |
| ATOM | 1662 | N | GLY | A | 209 | 20.540 | 14.284 | 60.822 | 1.00 | 36.80 | 7 |
| ATOM | 1663 | CA | GLY | A | 209 | 21.703 | 13.428 | 60.728 | 1.00 | 38.99 | 6 |
| ATOM | 1664 | C | GLY | A | 209 | 21.509 | 12.246 | 59.805 | 1.00 | 40.93 | 6 |
| ATOM | 1665 | O | GLY | A | 209 | 20.477 | 12.124 | 59.145 | 1.00 | 40.26 | 8 |
| ATOM | 1666 | N | GLU | A | 210 | 22.508 | 11.370 | 59.775 | 1.00 | 42.16 | 7 |
| ATOM | 1667 | CA | GLU | A | 210 | 22.492 | 10.185 | 58.930 | 1.00 | 43.30 | 6 |
| ATOM | 1668 | CB | GLU | A | 210 | 22.810 | 10.586 | 57.488 | 1.00 | 47.08 | 6 |
| ATOM | 1669 | CG | GLU | A | 210 | 22.826 | 9.453 | 56.478 | 1.00 | 53.90 | 6 |
| ATOM | 1670 | CD | GLU | A | 210 | 23.256 | 9.915 | 55.089 | 1.00 | 56.27 | 6 |
| ATOM | 1671 | OE1 | GLU | A | 210 | 24.412 | 10.371 | 54.941 | 1.00 | 56.19 | 8 |
| ATOM | 1672 | OE2 | GLU | A | 210 | 22.437 | 9.826 | 54.145 | 1.00 | 60.28 | 8 |
| ATOM | 1673 | C | GLU | A | 210 | 23.583 | 9.276 | 59.473 | 1.00 | 41.47 | 6 |
| ATOM | 1674 | O | GLU | A | 210 | 24.750 | 9.457 | 59.152 | 1.00 | 43.97 | 8 |
| ATOM | 1675 | N | GLY | A | 211 | 23.203 | 8.307 | 60.299 | 1.00 | 39.97 | 7 |
| ATOM | 1676 | CA | GLY | A | 211 | 24.181 | 7.405 | 60.885 | 1.00 | 37.34 | 6 |
| ATOM | 1677 | C | GLY | A | 211 | 24.642 | 7.952 | 62.224 | 1.00 | 37.84 | 6 |
| ATOM | 1678 | O | GLY | A | 211 | 23.820 | 8.408 | 63.019 | 1.00 | 37.30 | 8 |
| ATOM | 1679 | N | LYS | A | 212 | 25.948 | 7.910 | 62.485 | 1.00 | 38.52 | 7 |
| ATOM | 1680 | CA | LYS | A | 212 | 26.490 | 8.440 | 63.733 | 1.00 | 38.29 | 6 |
| ATOM | 1681 | CB | LYS | A | 212 | 28.020 | 8.359 | 63.731 | 1.00 | 40.54 | 6 |
| ATOM | 1682 | CG | LYS | A | 212 | 28.570 | 6.950 | 63.675 | 1.00 | 46.39 | 6 |
| ATOM | 1683 | CD | LYS | A | 212 | 28.149 | 6.147 | 64.910 | 1.00 | 51.59 | 6 |
| ATOM | 1684 | CE | LYS | A | 212 | 28.556 | 4.676 | 64.809 | 1.00 | 52.77 | 6 |
| ATOM | 1685 | NZ | LYS | A | 212 | 30.030 | 4.478 | 64.662 | 1.00 | 55.48 | 7 |
| ATOM | 1686 | C | LYS | A | 212 | 26.061 | 9.897 | 63.866 | 1.00 | 37.68 | 6 |
| ATOM | 1687 | O | LYS | A | 212 | 25.814 | 10.389 | 64.962 | 1.00 | 34.75 | 8 |
| ATOM | 1688 | N | GLY | A | 213 | 25.956 | 10.574 | 62.728 | 1.00 | 38.89 | 7 |
| ATOM | 1689 | CA | GLY | A | 213 | 25.577 | 11.975 | 62.724 | 1.00 | 43.58 | 6 |
| ATOM | 1690 | C | GLY | A | 213 | 24.126 | 12.295 | 63.020 | 1.00 | 43.99 | 6 |
| ATOM | 1691 | O | GLY | A | 213 | 23.737 | 13.464 | 63.024 | 1.00 | 44.67 | 8 |
| ATOM | 1692 | N | LYS | A | 214 | 23.321 | 11.268 | 63.265 | 1.00 | 46.02 | 7 |
| ATOM | 1693 | CA | LYS | A | 214 | 21.907 | 11.467 | 63.562 | 1.00 | 45.61 | 6 |
| ATOM | 1694 | CB | LYS | A | 214 | 21.168 | 10.130 | 63.469 | 1.00 | 47.77 | 6 |
| ATOM | 1695 | CG | LYS | A | 214 | 19.675 | 10.252 | 63.249 | 1.00 | 49.25 | 6 |
| ATOM | 1696 | CD | LYS | A | 214 | 19.078 | 8.901 | 62.911 | 1.00 | 51.64 | 6 |
| ATOM | 1697 | CE | LYS | A | 214 | 17.637 | 9.038 | 62.440 | 1.00 | 54.30 | 6 |
| ATOM | 1698 | NZ | LYS | A | 214 | 17.030 | 7.727 | 62.034 | 1.00 | 56.09 | 7 |
| ATOM | 1699 | C | LYS | A | 214 | 21.809 | 12.047 | 64.970 | 1.00 | 44.22 | 6 |
| ATOM | 1700 | O | LYS | A | 214 | 22.210 | 11.410 | 65.942 | 1.00 | 45.04 | 8 |
| ATOM | 1701 | N | GLY | A | 215 | 21.292 | 13.266 | 65.074 | 1.00 | 42.89 | 7 |
| ATOM | 1702 | CA | GLY | A | 215 | 21.193 | 13.904 | 66.373 | 1.00 | 40.20 | 6 |
| ATOM | 1703 | C | GLY | A | 215 | 22.295 | 14.931 | 66.600 | 1.00 | 39.90 | 6 |
| ATOM | 1704 | O | GLY | A | 215 | 22.356 | 15.548 | 67.668 | 1.00 | 40.12 | 8 |
| ATOM | 1705 | N | TYR | A | 216 | 23.175 | 15.111 | 65.612 | 1.00 | 38.49 | 7 |
| ATOM | 1706 | CA | TYR | A | 216 | 24.261 | 16.086 | 65.726 | 1.00 | 35.91 | 6 |
| ATOM | 1707 | CB | TYR | A | 216 | 25.632 | 15.421 | 65.618 | 1.00 | 36.47 | 6 |
| ATOM | 1708 | CG | TYR | A | 216 | 25.935 | 14.461 | 66.738 | 1.00 | 39.54 | 6 |
| ATOM | 1709 | CD1 | TYR | A | 216 | 25.296 | 13.220 | 66.810 | 1.00 | 40.62 | 6 |
| ATOM | 1710 | CE1 | TYR | A | 216 | 25.561 | 12.333 | 67.849 | 1.00 | 41.58 | 6 |
| ATOM | 1711 | CD2 | TYR | A | 216 | 26.852 | 14.795 | 67.739 | 1.00 | 39.20 | 6 |
| ATOM | 1712 | CE2 | TYR | A | 216 | 27.124 | 13.915 | 68.786 | 1.00 | 40.87 | 6 |
| ATOM | 1713 | CZ | TYR | A | 216 | 26.475 | 12.685 | 68.833 | 1.00 | 41.86 | 6 |
| ATOM | 1714 | OH | TYR | A | 216 | 26.743 | 11.802 | 69.852 | 1.00 | 43.04 | 8 |
| ATOM | 1715 | C | TYR | A | 216 | 24.182 | 17.215 | 64.709 | 1.00 | 34.21 | 6 |
| ATOM | 1716 | O | TYR | A | 216 | 25.194 | 17.832 | 64.375 | 1.00 | 33.37 | 8 |

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Figure 17-27

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 1717 | N | ASN A 217 | 22.976 | 17.471 | 64.212 | 1.00 | 33.83 | 7 |
| ATOM | 1718 | CA | ASN A 217 | 22.726 | 18.558 | 63.267 | 1.00 | 30.20 | 6 |
| ATOM | 1719 | CB | ASN A 217 | 22.699 | 18.057 | 61.823 | 1.00 | 27.74 | 6 |
| ATOM | 1720 | CG | ASN A 217 | 22.457 | 19.177 | 60.826 | 1.00 | 25.61 | 6 |
| ATOM | 1721 | OD1 | ASN A 217 | 21.354 | 19.705 | 60.719 | 1.00 | 25.00 | 8 |
| ATOM | 1722 | ND2 | ASN A 217 | 23.501 | 19.558 | 60.103 | 1.00 | 30.43 | 7 |
| ATOM | 1723 | C | ASN A 217 | 21.369 | 19.116 | 63.645 | 1.00 | 29.09 | 6 |
| ATOM | 1724 | O | ASN A 217 | 20.433 | 18.351 | 63.885 | 1.00 | 26.93 | 8 |
| ATOM | 1725 | N | LEU A 218 | 21.263 | 20.440 | 63.710 | 1.00 | 27.19 | 7 |
| ATOM | 1726 | CA | LEU A 218 | 20.010 | 21.071 | 64.089 | 1.00 | 25.33 | 6 |
| ATOM | 1727 | CB | LEU A 218 | 20.026 | 21.379 | 65.590 | 1.00 | 23.23 | 6 |
| ATOM | 1728 | CG | LEU A 218 | 18.729 | 21.704 | 66.346 | 1.00 | 21.00 | 6 |
| ATOM | 1729 | CD1 | LEU A 218 | 19.100 | 22.313 | 67.695 | 1.00 | 18.62 | 6 |
| ATOM | 1730 | CD2 | LEU A 218 | 17.872 | 22.675 | 65.583 | 1.00 | 18.48 | 6 |
| ATOM | 1731 | C | LEU A 218 | 19.785 | 22.368 | 63.325 | 1.00 | 25.04 | 6 |
| ATOM | 1732 | O | LEU A 218 | 20.596 | 23.287 | 63.415 | 1.00 | 25.23 | 8 |
| ATOM | 1733 | N | ASN A 219 | 18.681 | 22.436 | 62.584 | 1.00 | 28.44 | 7 |
| ATOM | 1734 | CA | ASN A 219 | 18.310 | 23.636 | 61.829 | 1.00 | 28.76 | 6 |
| ATOM | 1735 | CB | ASN A 219 | 17.809 | 23.298 | 60.417 | 1.00 | 25.69 | 6 |
| ATOM | 1736 | CG | ASN A 219 | 18.748 | 22.408 | 59.646 | 1.00 | 26.10 | 6 |
| ATOM | 1737 | OD1 | ASN A 219 | 19.927 | 22.708 | 59.505 | 1.00 | 28.53 | 8 |
| ATOM | 1738 | ND2 | ASN A 219 | 18.220 | 21.311 | 59.114 | 1.00 | 26.97 | 7 |
| ATOM | 1739 | C | ASN A 219 | 17.129 | 24.248 | 62.582 | 1.00 | 31.96 | 6 |
| ATOM | 1740 | O | ASN A 219 | 16.373 | 23.539 | 63.246 | 1.00 | 34.84 | 8 |
| ATOM | 1741 | N | ILE A 220 | 16.952 | 25.556 | 62.472 | 1.00 | 32.96 | 7 |
| ATOM | 1742 | CA | ILE A 220 | 15.826 | 26.196 | 63.129 | 1.00 | 32.50 | 6 |
| ATOM | 1743 | CB | ILE A 220 | 16.259 | 27.037 | 64.350 | 1.00 | 32.32 | 6 |
| ATOM | 1744 | CG2 | ILE A 220 | 15.029 | 27.644 | 65.014 | 1.00 | 29.46 | 6 |
| ATOM | 1745 | CG1 | ILE A 220 | 16.978 | 26.160 | 65.374 | 1.00 | 29.65 | 6 |
| ATOM | 1746 | CD1 | ILE A 220 | 16.080 | 25.138 | 66.027 | 1.00 | 28.65 | 6 |
| ATOM | 1747 | C | ILE A 220 | 15.140 | 27.106 | 62.123 | 1.00 | 35.36 | 6 |
| ATOM | 1748 | O | ILE A 220 | 15.469 | 28.290 | 62.009 | 1.00 | 35.52 | 8 |
| ATOM | 1749 | N | PRO A 221 | 14.185 | 26.553 | 61.359 | 1.00 | 36.87 | 7 |
| ATOM | 1750 | CD | PRO A 221 | 13.718 | 25.158 | 61.359 | 1.00 | 35.12 | 6 |
| ATOM | 1751 | CA | PRO A 221 | 13.445 | 27.318 | 60.356 | 1.00 | 35.41 | 6 |
| ATOM | 1752 | CB | PRO A 221 | 12.509 | 26.262 | 59.767 | 1.00 | 35.68 | 6 |
| ATOM | 1753 | CG | PRO A 221 | 13.319 | 24.992 | 59.911 | 1.00 | 33.86 | 6 |
| ATOM | 1754 | C | PRO A 221 | 12.696 | 28.437 | 61.053 | 1.00 | 34.37 | 6 |
| ATOM | 1755 | O | PRO A 221 | 12.014 | 28.199 | 62.043 | 1.00 | 38.79 | 8 |
| ATOM | 1756 | N | LEU A 222 | 12.815 | 29.655 | 60.547 | 1.00 | 34.76 | 7 |
| ATOM | 1757 | CA | LEU A 222 | 12.138 | 30.796 | 61.166 | 1.00 | 33.87 | 6 |
| ATOM | 1758 | CB | LEU A 222 | 13.173 | 31.735 | 61.798 | 1.00 | 35.13 | 6 |
| ATOM | 1759 | CG | LEU A 222 | 14.104 | 31.163 | 62.876 | 1.00 | 33.07 | 6 |
| ATOM | 1760 | CD1 | LEU A 222 | 15.234 | 32.150 | 63.154 | 1.00 | 34.04 | 6 |
| ATOM | 1761 | CD2 | LEU A 222 | 13.312 | 30.856 | 64.141 | 1.00 | 32.39 | 6 |
| ATOM | 1762 | C | LEU A 222 | 11.287 | 31.567 | 60.157 | 1.00 | 32.15 | 6 |
| ATOM | 1763 | O | LEU A 222 | 11.669 | 31.740 | 59.000 | 1.00 | 31.32 | 8 |
| ATOM | 1764 | N | PRO A 223 | 10.127 | 32.060 | 60.601 | 1.00 | 30.97 | 7 |
| ATOM | 1765 | CD | PRO A 223 | 9.606 | 31.913 | 61.972 | 1.00 | 32.34 | 6 |
| ATOM | 1766 | CA | PRO A 223 | 9.173 | 32.818 | 59.789 | 1.00 | 30.55 | 6 |
| ATOM | 1767 | CB | PRO A 223 | 7.957 | 32.893 | 60.702 | 1.00 | 29.44 | 6 |
| ATOM | 1768 | CG | PRO A 223 | 8.626 | 33.068 | 62.046 | 1.00 | 31.02 | 6 |
| ATOM | 1769 | C | PRO A 223 | 9.645 | 34.205 | 59.366 | 1.00 | 29.20 | 6 |
| ATOM | 1770 | O | PRO A 223 | 10.694 | 34.680 | 59.796 | 1.00 | 31.95 | 8 |
| ATOM | 1771 | N | LYS A 224 | 8.841 | 34.841 | 58.521 | 1.00 | 26.14 | 7 |
| ATOM | 1772 | CA | LYS A 224 | 9.115 | 36.172 | 58.026 | 1.00 | 23.54 | 6 |
| ATOM | 1773 | CB | LYS A 224 | 8.285 | 36.443 | 56.766 | 1.00 | 24.71 | 6 |
| ATOM | 1774 | CG | LYS A 224 | 8.563 | 35.500 | 55.619 | 1.00 | 23.83 | 6 |
| ATOM | 1775 | CD | LYS A 224 | 7.737 | 35.800 | 54.394 | 1.00 | 20.59 | 6 |
| ATOM | 1776 | CE | LYS A 224 | 8.065 | 34.769 | 53.329 | 1.00 | 27.03 | 6 |
| ATOM | 1777 | NZ | LYS A 224 | 7.198 | 34.849 | 52.122 | 1.00 | 30.48 | 7 |
| ATOM | 1778 | C | LYS A 224 | 8.702 | 37.151 | 59.111 | 1.00 | 25.48 | 6 |
| ATOM | 1779 | O | LYS A 224 | 7.999 | 36.780 | 60.055 | 1.00 | 22.67 | 8 |
| ATOM | 1780 | N | GLY A 225 | 9.124 | 38.404 | 58.960 | 1.00 | 26.88 | 7 |
| ATOM | 1781 | CA | GLY A 225 | 8.777 | 39.432 | 59.925 | 1.00 | 29.80 | 6 |
| ATOM | 1782 | C | GLY A 225 | 9.396 | 39.188 | 61.286 | 1.00 | 32.96 | 6 |

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Figure 17-28

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 1783 | O | GLY A 225 | 9.068 | 39.861 | 62.271 | 1.00 | 31.20 | 8 |
| ATOM | 1784 | N | LEU A 226 | 10.299 | 38.216 | 61.338 | 1.00 | 32.86 | 7 |
| ATOM | 1785 | CA | LEU A 226 | 10.975 | 37.877 | 62.575 | 1.00 | 34.55 | 6 |
| ATOM | 1786 | CB | LEU A 226 | 12.149 | 36.958 | 62.255 | 1.00 | 34.46 | 6 |
| ATOM | 1787 | CG | LEU A 226 | 12.982 | 36.413 | 63.407 | 1.00 | 34.48 | 6 |
| ATOM | 1788 | CD1 | LEU A 226 | 12.146 | 35.425 | 64.212 | 1.00 | 33.18 | 6 |
| ATOM | 1789 | CD2 | LEU A 226 | 14.207 | 35.724 | 62.847 | 1.00 | 31.39 | 6 |
| ATOM | 1790 | C | LEU A 226 | 11.481 | 39.160 | 63.255 | 1.00 | 36.29 | 6 |
| ATOM | 1791 | O | LEU A 226 | 12.156 | 39.970 | 62.613 | 1.00 | 33.87 | 8 |
| ATOM | 1792 | N | ASN A 227 | 11.131 | 39.358 | 64.531 | 1.00 | 37.31 | 7 |
| ATOM | 1793 | CA | ASN A 227 | 11.592 | 40.536 | 65.279 | 1.00 | 37.26 | 6 |
| ATOM | 1794 | CB | ASN A 227 | 10.444 | 41.212 | 66.053 | 1.00 | 35.57 | 6 |
| ATOM | 1795 | CG | ASN A 227 | 9.920 | 40.368 | 67.208 | 1.00 | 36.07 | 6 |
| ATOM | 1796 | OD1 | ASN A 227 | 10.678 | 39.940 | 68.089 | 1.00 | 35.08 | 8 |
| ATOM | 1797 | ND2 | ASN A 227 | 8.611 | 40.143 | 67.218 | 1.00 | 32.33 | 7 |
| ATOM | 1798 | C | ASN A 227 | 12.688 | 40.096 | 66.250 | 1.00 | 37.95 | 6 |
| ATOM | 1799 | O | ASN A 227 | 12.869 | 38.890 | 66.473 | 1.00 | 37.08 | 8 |
| ATOM | 1800 | N | ASP A 228 | 13.403 | 41.063 | 66.832 | 1.00 | 36.07 | 7 |
| ATOM | 1801 | CA | ASP A 228 | 14.505 | 40.754 | 67.751 | 1.00 | 37.63 | 6 |
| ATOM | 1802 | CB | ASP A 228 | 14.996 | 42.007 | 68.486 | 1.00 | 36.48 | 6 |
| ATOM | 1803 | CG | ASP A 228 | 15.480 | 43.088 | 67.545 | 1.00 | 37.52 | 6 |
| ATOM | 1804 | OD1 | ASP A 228 | 15.936 | 42.752 | 66.427 | 1.00 | 35.28 | 8 |
| ATOM | 1805 | OD2 | ASP A 228 | 15.426 | 44.274 | 67.937 | 1.00 | 39.01 | 8 |
| ATOM | 1806 | C | ASP A 228 | 14.204 | 39.678 | 68.783 | 1.00 | 37.56 | 6 |
| ATOM | 1807 | O | ASP A 228 | 14.921 | 38.678 | 68.869 | 1.00 | 39.53 | 8 |
| ATOM | 1808 | N | ASN A 229 | 13.155 | 39.889 | 69.572 | 1.00 | 38.37 | 7 |
| ATOM | 1809 | CA | ASN A 229 | 12.766 | 38.935 | 70.605 | 1.00 | 37.49 | 6 |
| ATOM | 1810 | CB | ASN A 229 | 11.422 | 39.352 | 71.200 | 1.00 | 37.38 | 6 |
| ATOM | 1811 | CG | ASN A 229 | 11.490 | 40.709 | 71.877 | 1.00 | 40.47 | 6 |
| ATOM | 1812 | OD1 | ASN A 229 | 12.041 | 40.840 | 72.973 | 1.00 | 41.76 | 8 |
| ATOM | 1813 | ND2 | ASN A 229 | 10.960 | 41.735 | 71.212 | 1.00 | 36.50 | 7 |
| ATOM | 1814 | C | ASN A 229 | 12.680 | 37.530 | 70.017 | 1.00 | 37.64 | 6 |
| ATOM | 1815 | O | ASN A 229 | 13.446 | 36.634 | 70.395 | 1.00 | 35.76 | 8 |
| ATOM | 1816 | N | GLU A 230 | 11.758 | 37.351 | 69.076 | 1.00 | 36.01 | 7 |
| ATOM | 1817 | CA | GLU A 230 | 11.574 | 36.062 | 68.425 | 1.00 | 34.74 | 6 |
| ATOM | 1818 | CB | GLU A 230 | 10.753 | 36.242 | 67.153 | 1.00 | 35.55 | 6 |
| ATOM | 1819 | CG | GLU A 230 | 9.382 | 36.820 | 67.407 | 1.00 | 36.95 | 6 |
| ATOM | 1820 | CD | GLU A 230 | 8.580 | 36.960 | 66.144 | 1.00 | 35.30 | 6 |
| ATOM | 1821 | OE1 | GLU A 230 | 9.042 | 37.670 | 65.229 | 1.00 | 36.98 | 8 |
| ATOM | 1822 | OE2 | GLU A 230 | 7.490 | 36.361 | 66.065 | 1.00 | 36.71 | 8 |
| ATOM | 1823 | C | GLU A 230 | 12.916 | 35.421 | 68.082 | 1.00 | 33.92 | 6 |
| ATOM | 1824 | O | GLU A 230 | 13.143 | 34.238 | 68.346 | 1.00 | 32.74 | 8 |
| ATOM | 1825 | N | PHE A 231 | 13.804 | 36.207 | 67.487 | 1.00 | 32.03 | 7 |
| ATOM | 1826 | CA | PHE A 231 | 15.116 | 35.712 | 67.123 | 1.00 | 30.55 | 6 |
| ATOM | 1827 | CB | PHE A 231 | 15.932 | 36.821 | 66.460 | 1.00 | 33.86 | 6 |
| ATOM | 1828 | CG | PHE A 231 | 17.295 | 36.381 | 66.012 | 1.00 | 36.97 | 6 |
| ATOM | 1829 | CD1 | PHE A 231 | 17.438 | 35.334 | 65.102 | 1.00 | 40.41 | 6 |
| ATOM | 1830 | CD2 | PHE A 231 | 18.436 | 37.021 | 66.480 | 1.00 | 36.58 | 6 |
| ATOM | 1831 | CE1 | PHE A 231 | 18.709 | 34.932 | 64.661 | 1.00 | 43.00 | 6 |
| ATOM | 1832 | CE2 | PHE A 231 | 19.711 | 36.632 | 66.049 | 1.00 | 39.07 | 6 |
| ATOM | 1833 | CZ | PHE A 231 | 19.849 | 35.586 | 65.137 | 1.00 | 40.52 | 6 |
| ATOM | 1834 | C | PHE A 231 | 15.835 | 35.232 | 68.376 | 1.00 | 30.63 | 6 |
| ATOM | 1835 | O | PHE A 231 | 16.177 | 34.042 | 68.497 | 1.00 | 29.66 | 8 |
| ATOM | 1836 | N | LEU A 232 | 16.049 | 36.162 | 69.310 | 1.00 | 24.94 | 7 |
| ATOM | 1837 | CA | LEU A 232 | 16.742 | 35.857 | 70.556 | 1.00 | 22.82 | 6 |
| ATOM | 1838 | CB | LEU A 232 | 16.724 | 37.084 | 71.468 | 1.00 | 24.96 | 6 |
| ATOM | 1839 | CG | LEU A 232 | 17.507 | 38.282 | 70.890 | 1.00 | 29.34 | 6 |
| ATOM | 1840 | CD1 | LEU A 232 | 17.316 | 39.549 | 71.746 | 1.00 | 24.38 | 6 |
| ATOM | 1841 | CD2 | LEU A 232 | 18.991 | 37.903 | 70.787 | 1.00 | 27.39 | 6 |
| ATOM | 1842 | C | LEU A 232 | 16.150 | 34.638 | 71.261 | 1.00 | 22.44 | 6 |
| ATOM | 1843 | O | LEU A 232 | 16.882 | 33.793 | 71.767 | 1.00 | 20.37 | 8 |
| ATOM | 1844 | N | PHE A 233 | 14.825 | 34.552 | 71.289 | 1.00 | 24.81 | 7 |
| ATOM | 1845 | CA | PHE A 233 | 14.131 | 33.422 | 71.905 | 1.00 | 25.81 | 6 |
| ATOM | 1846 | CB | PHE A 233 | 12.623 | 33.535 | 71.641 | 1.00 | 24.37 | 6 |
| ATOM | 1847 | CG | PHE A 233 | 11.811 | 32.373 | 72.157 | 1.00 | 24.18 | 6 |
| ATOM | 1848 | CD1 | PHE A 233 | 11.491 | 32.264 | 73.503 | 1.00 | 25.59 | 6 |

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Figure 17-29

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1849 | CD2 | PHE | A | 233 | 11.339 | 31.397 | 71.284 | 1.00 | 25.75 | 6 |
| ATOM | 1850 | CE1 | PHE | A | 233 | 10.698 | 31.198 | 73.974 | 1.00 | 25.33 | 6 |
| ATOM | 1851 | CE2 | PHE | A | 233 | 10.548 | 30.327 | 71.747 | 1.00 | 24.02 | 6 |
| ATOM | 1852 | CZ | PHE | A | 233 | 10.228 | 30.232 | 73.093 | 1.00 | 22.77 | 6 |
| ATOM | 1853 | C | PHE | A | 233 | 14.661 | 32.133 | 71.275 | 1.00 | 26.64 | 6 |
| ATOM | 1854 | O | PHE | A | 233 | 15.094 | 31.209 | 71.971 | 1.00 | 28.34 | 8 |
| ATOM | 1855 | N | ALA | A | 234 | 14.624 | 32.087 | 69.949 | 1.00 | 27.27 | 7 |
| ATOM | 1856 | CA | ALA | A | 234 | 15.080 | 30.921 | 69.209 | 1.00 | 30.24 | 6 |
| ATOM | 1857 | CB | ALA | A | 234 | 14.797 | 31.107 | 67.720 | 1.00 | 33.38 | 6 |
| ATOM | 1858 | C | ALA | A | 234 | 16.563 | 30.645 | 69.433 | 1.00 | 30.76 | 6 |
| ATOM | 1859 | O | ALA | A | 234 | 16.981 | 29.491 | 69.488 | 1.00 | 30.04 | 8 |
| ATOM | 1860 | N | LEU | A | 235 | 17.363 | 31.695 | 69.563 | 1.00 | 31.84 | 7 |
| ATOM | 1861 | CA | LEU | A | 235 | 18.789 | 31.486 | 69.790 | 1.00 | 32.83 | 6 |
| ATOM | 1862 | CB | LEU | A | 235 | 19.548 | 32.819 | 69.703 | 1.00 | 34.12 | 6 |
| ATOM | 1863 | CG | LEU | A | 235 | 21.039 | 32.745 | 69.316 | 1.00 | 36.33 | 6 |
| ATOM | 1864 | CD1 | LEU | A | 235 | 21.625 | 34.156 | 69.205 | 1.00 | 36.44 | 6 |
| ATOM | 1865 | CD2 | LEU | A | 235 | 21.803 | 31.939 | 70.330 | 1.00 | 35.64 | 6 |
| ATOM | 1866 | C | LEU | A | 235 | 18.970 | 30.846 | 71.176 | 1.00 | 30.75 | 6 |
| ATOM | 1867 | O | LEU | A | 235 | 19.648 | 29.835 | 71.312 | 1.00 | 30.12 | 8 |
| ATOM | 1868 | N | GLU | A | 236 | 18.347 | 31.435 | 72.192 | 1.00 | 29.03 | 7 |
| ATOM | 1869 | CA | GLU | A | 236 | 18.418 | 30.931 | 73.561 | 1.00 | 33.32 | 6 |
| ATOM | 1870 | CB | GLU | A | 236 | 17.479 | 31.730 | 74.452 | 1.00 | 35.06 | 6 |
| ATOM | 1871 | CG | GLU | A | 236 | 17.843 | 33.176 | 74.635 | 1.00 | 42.35 | 6 |
| ATOM | 1872 | CD | GLU | A | 236 | 16.610 | 34.022 | 74.843 | 1.00 | 47.12 | 6 |
| ATOM | 1873 | OE1 | GLU | A | 236 | 15.686 | 33.557 | 75.556 | 1.00 | 48.91 | 8 |
| ATOM | 1874 | OE2 | GLU | A | 236 | 16.572 | 35.150 | 74.297 | 1.00 | 49.07 | 8 |
| ATOM | 1875 | C | GLU | A | 236 | 17.988 | 29.473 | 73.639 | 1.00 | 34.65 | 6 |
| ATOM | 1876 | O | GLU | A | 236 | 18.715 | 28.593 | 74.116 | 1.00 | 30.43 | 8 |
| ATOM | 1877 | N | LYS | A | 237 | 16.767 | 29.250 | 73.176 | 1.00 | 35.67 | 7 |
| ATOM | 1878 | CA | LYS | A | 237 | 16.138 | 27.943 | 73.175 | 1.00 | 35.51 | 6 |
| ATOM | 1879 | CB | LYS | A | 237 | 14.791 | 28.060 | 72.452 | 1.00 | 37.01 | 6 |
| ATOM | 1880 | CG | LYS | A | 237 | 13.745 | 27.032 | 72.848 | 1.00 | 39.65 | 6 |
| ATOM | 1881 | CD | LYS | A | 237 | 12.712 | 27.605 | 73.821 | 1.00 | 40.66 | 6 |
| ATOM | 1882 | CE | LYS | A | 237 | 13.312 | 28.054 | 75.153 | 1.00 | 40.58 | 6 |
| ATOM | 1883 | NZ | LYS | A | 237 | 12.250 | 28.556 | 76.083 | 1.00 | 32.05 | 7 |
| ATOM | 1884 | C | LYS | A | 237 | 17.025 | 26.891 | 72.485 | 1.00 | 35.07 | 6 |
| ATOM | 1885 | O | LYS | A | 237 | 17.315 | 25.833 | 73.061 | 1.00 | 30.60 | 8 |
| ATOM | 1886 | N | SER | A | 238 | 17.455 | 27.200 | 71.259 | 1.00 | 33.59 | 7 |
| ATOM | 1887 | CA | SER | A | 238 | 18.279 | 26.293 | 70.452 | 1.00 | 32.18 | 6 |
| ATOM | 1888 | CB | SER | A | 238 | 18.453 | 26.867 | 69.042 | 1.00 | 32.01 | 6 |
| ATOM | 1889 | OG | SER | A | 238 | 19.014 | 28.168 | 69.075 | 1.00 | 37.80 | 8 |
| ATOM | 1890 | C | SER | A | 238 | 19.650 | 25.928 | 71.032 | 1.00 | 31.94 | 6 |
| ATOM | 1891 | O | SER | A | 238 | 20.064 | 24.758 | 70.990 | 1.00 | 26.88 | 8 |
| ATOM | 1892 | N | LEU | A | 239 | 20.357 | 26.920 | 71.564 | 1.00 | 31.19 | 7 |
| ATOM | 1893 | CA | LEU | A | 239 | 21.660 | 26.650 | 72.147 | 1.00 | 30.82 | 6 |
| ATOM | 1894 | CB | LEU | A | 239 | 22.293 | 27.914 | 72.720 | 1.00 | 28.03 | 6 |
| ATOM | 1895 | CG | LEU | A | 239 | 22.650 | 29.087 | 71.817 | 1.00 | 24.31 | 6 |
| ATOM | 1896 | CD1 | LEU | A | 239 | 23.210 | 30.189 | 72.695 | 1.00 | 24.63 | 6 |
| ATOM | 1897 | CD2 | LEU | A | 239 | 23.663 | 28.681 | 70.770 | 1.00 | 23.11 | 6 |
| ATOM | 1898 | C | LEU | A | 239 | 21.463 | 25.666 | 73.275 | 1.00 | 31.99 | 6 |
| ATOM | 1899 | O | LEU | A | 239 | 22.279 | 24.764 | 73.473 | 1.00 | 32.57 | 8 |
| ATOM | 1900 | N | GLU | A | 240 | 20.367 | 25.835 | 74.009 | 1.00 | 33.86 | 7 |
| ATOM | 1901 | CA | GLU | A | 240 | 20.094 | 24.965 | 75.136 | 1.00 | 38.61 | 6 |
| ATOM | 1902 | CB | GLU | A | 240 | 18.799 | 25.369 | 75.842 | 1.00 | 43.21 | 6 |
| ATOM | 1903 | CG | GLU | A | 240 | 18.500 | 24.468 | 77.045 | 1.00 | 53.52 | 6 |
| ATOM | 1904 | CD | GLU | A | 240 | 19.677 | 24.383 | 78.022 | 1.00 | 56.39 | 6 |
| ATOM | 1905 | OE1 | GLU | A | 240 | 19.969 | 25.399 | 78.701 | 1.00 | 57.81 | 8 |
| ATOM | 1906 | OE2 | GLU | A | 240 | 20.318 | 23.304 | 78.093 | 1.00 | 55.12 | 8 |
| ATOM | 1907 | C | GLU | A | 240 | 20.033 | 23.507 | 74.722 | 1.00 | 39.28 | 6 |
| ATOM | 1908 | O | GLU | A | 240 | 20.532 | 22.630 | 75.437 | 1.00 | 38.83 | 8 |
| ATOM | 1909 | N | ILE | A | 241 | 19.423 | 23.252 | 73.567 | 1.00 | 40.74 | 7 |
| ATOM | 1910 | CA | ILE | A | 241 | 19.310 | 21.896 | 73.035 | 1.00 | 38.08 | 6 |
| ATOM | 1911 | CB | ILE | A | 241 | 18.465 | 21.871 | 71.734 | 1.00 | 33.57 | 6 |
| ATOM | 1912 | CG2 | ILE | A | 241 | 18.536 | 20.506 | 71.086 | 1.00 | 31.39 | 6 |
| ATOM | 1913 | CG1 | ILE | A | 241 | 17.012 | 22.226 | 72.056 | 1.00 | 31.06 | 6 |
| ATOM | 1914 | CD1 | ILE | A | 241 | 16.147 | 22.478 | 70.843 | 1.00 | 27.53 | 6 |

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Figure 17-30

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 1915 | C | ILE A 241 | 20.713 | 21.372 | 72.747 | 1.00 | 39.56 | 6 |
| ATOM | 1916 | O | ILE A 241 | 20.984 | 20.189 | 72.936 | 1.00 | 40.82 | 8 |
| ATOM | 1917 | N | VAL A 242 | 21.605 | 22.254 | 72.299 | 1.00 | 41.93 | 7 |
| ATOM | 1918 | CA | VAL A 242 | 22.979 | 21.842 | 72.015 | 1.00 | 45.09 | 6 |
| ATOM | 1919 | CB | VAL A 242 | 23.808 | 22.959 | 71.329 | 1.00 | 45.76 | 6 |
| ATOM | 1920 | CG1 | VAL A 242 | 25.242 | 22.479 | 71.116 | 1.00 | 43.09 | 6 |
| ATOM | 1921 | CG2 | VAL A 242 | 23.182 | 23.334 | 69.991 | 1.00 | 46.41 | 6 |
| ATOM | 1922 | C | VAL A 242 | 23.698 | 21.453 | 73.300 | 1.00 | 45.69 | 6 |
| ATOM | 1923 | O | VAL A 242 | 24.191 | 20.331 | 73.423 | 1.00 | 46.30 | 8 |
| ATOM | 1924 | N | LYS A 243 | 23.750 | 22.373 | 74.259 | 1.00 | 44.60 | 7 |
| ATOM | 1925 | CA | LYS A 243 | 24.427 | 22.088 | 75.513 | 1.00 | 46.96 | 6 |
| ATOM | 1926 | CB | LYS A 243 | 24.214 | 23.217 | 76.527 | 1.00 | 49.49 | 6 |
| ATOM | 1927 | CG | LYS A 243 | 25.061 | 23.023 | 77.795 | 1.00 | 54.90 | 6 |
| ATOM | 1928 | CD | LYS A 243 | 24.652 | 23.934 | 78.939 | 1.00 | 58.95 | 6 |
| ATOM | 1929 | CE | LYS A 243 | 24.782 | 25.399 | 78.577 | 1.00 | 64.13 | 6 |
| ATOM | 1930 | NZ | LYS A 243 | 24.274 | 26.283 | 79.676 | 1.00 | 66.93 | 7 |
| ATOM | 1931 | C | LYS A 243 | 23.965 | 20.767 | 76.135 | 1.00 | 47.06 | 6 |
| ATOM | 1932 | O | LYS A 243 | 24.735 | 20.113 | 76.845 | 1.00 | 46.39 | 8 |
| ATOM | 1933 | N | GLU A 244 | 22.716 | 20.380 | 75.878 | 1.00 | 47.51 | 7 |
| ATOM | 1934 | CA | GLU A 244 | 22.172 | 19.136 | 76.429 | 1.00 | 51.33 | 6 |
| ATOM | 1935 | CB | GLU A 244 | 20.650 | 19.061 | 76.259 | 1.00 | 54.49 | 6 |
| ATOM | 1936 | CG | GLU A 244 | 19.843 | 20.199 | 76.842 | 1.00 | 62.61 | 6 |
| ATOM | 1937 | CD | GLU A 244 | 18.360 | 20.089 | 76.489 | 1.00 | 65.15 | 6 |
| ATOM | 1938 | OE1 | GLU A 244 | 17.572 | 20.980 | 76.888 | 1.00 | 66.49 | 8 |
| ATOM | 1939 | OE2 | GLU A 244 | 17.986 | 19.108 | 75.807 | 1.00 | 64.82 | 8 |
| ATOM | 1940 | C | GLU A 244 | 22.745 | 17.936 | 75.698 | 1.00 | 50.17 | 6 |
| ATOM | 1941 | O | GLU A 244 | 22.866 | 16.846 | 76.259 | 1.00 | 51.54 | 8 |
| ATOM | 1942 | N | VAL A 245 | 23.104 | 18.148 | 74.441 | 1.00 | 47.70 | 7 |
| ATOM | 1943 | CA | VAL A 245 | 23.587 | 17.063 | 73.611 | 1.00 | 45.43 | 6 |
| ATOM | 1944 | CB | VAL A 245 | 22.704 | 16.980 | 72.336 | 1.00 | 48.47 | 6 |
| ATOM | 1945 | CG1 | VAL A 245 | 23.082 | 15.765 | 71.499 | 1.00 | 51.87 | 6 |
| ATOM | 1946 | CG2 | VAL A 245 | 21.226 | 16.934 | 72.731 | 1.00 | 45.65 | 6 |
| ATOM | 1947 | C | VAL A 245 | 25.056 | 17.070 | 73.185 | 1.00 | 43.01 | 6 |
| ATOM | 1948 | O | VAL A 245 | 25.620 | 16.005 | 72.946 | 1.00 | 39.28 | 8 |
| ATOM | 1949 | N | PHE A 246 | 25.682 | 18.245 | 73.109 | 1.00 | 40.53 | 7 |
| ATOM | 1950 | CA | PHE A 246 | 27.063 | 18.321 | 72.633 | 1.00 | 38.56 | 6 |
| ATOM | 1951 | CB | PHE A 246 | 27.023 | 18.700 | 71.154 | 1.00 | 36.85 | 6 |
| ATOM | 1952 | CG | PHE A 246 | 28.315 | 18.487 | 70.415 | 1.00 | 36.46 | 6 |
| ATOM | 1953 | CD1 | PHE A 246 | 28.749 | 17.201 | 70.098 | 1.00 | 32.95 | 6 |
| ATOM | 1954 | CD2 | PHE A 246 | 29.064 | 19.582 | 69.967 | 1.00 | 35.51 | 6 |
| ATOM | 1955 | CE1 | PHE A 246 | 29.903 | 17.004 | 69.337 | 1.00 | 33.80 | 6 |
| ATOM | 1956 | CE2 | PHE A 246 | 30.222 | 19.397 | 69.206 | 1.00 | 34.46 | 6 |
| ATOM | 1957 | CZ | PHE A 246 | 30.640 | 18.103 | 68.889 | 1.00 | 35.54 | 6 |
| ATOM | 1958 | C | PHE A 246 | 27.970 | 19.311 | 73.371 | 1.00 | 40.83 | 6 |
| ATOM | 1959 | O | PHE A 246 | 27.613 | 20.478 | 73.549 | 1.00 | 40.32 | 8 |
| ATOM | 1960 | N | GLU A 247 | 29.141 | 18.839 | 73.802 | 1.00 | 42.54 | 7 |
| ATOM | 1961 | CA | GLU A 247 | 30.128 | 19.695 | 74.467 | 1.00 | 43.93 | 6 |
| ATOM | 1962 | CB | GLU A 247 | 30.655 | 19.075 | 75.770 | 1.00 | 45.67 | 6 |
| ATOM | 1963 | CG | GLU A 247 | 29.763 | 19.243 | 77.005 | 1.00 | 51.63 | 6 |
| ATOM | 1964 | CD | GLU A 247 | 28.478 | 18.424 | 76.962 | 1.00 | 57.42 | 6 |
| ATOM | 1965 | OE1 | GLU A 247 | 27.645 | 18.644 | 76.058 | 1.00 | 62.12 | 8 |
| ATOM | 1966 | OE2 | GLU A 247 | 28.296 | 17.557 | 77.845 | 1.00 | 59.43 | 8 |
| ATOM | 1967 | C | GLU A 247 | 31.268 | 19.839 | 73.464 | 1.00 | 43.62 | 6 |
| ATOM | 1968 | O | GLU A 247 | 32.077 | 18.931 | 73.294 | 1.00 | 44.25 | 8 |
| ATOM | 1969 | N | PRO A 248 | 31.342 | 20.988 | 72.780 | 1.00 | 43.65 | 7 |
| ATOM | 1970 | CD | PRO A 248 | 30.439 | 22.143 | 72.863 | 1.00 | 42.73 | 6 |
| ATOM | 1971 | CA | PRO A 248 | 32.371 | 21.260 | 71.779 | 1.00 | 43.28 | 6 |
| ATOM | 1972 | CB | PRO A 248 | 31.802 | 22.480 | 71.042 | 1.00 | 43.03 | 6 |
| ATOM | 1973 | CG | PRO A 248 | 30.317 | 22.474 | 71.415 | 1.00 | 43.02 | 6 |
| ATOM | 1974 | C | PRO A 248 | 33.759 | 21.552 | 72.331 | 1.00 | 43.37 | 6 |
| ATOM | 1975 | O | PRO A 248 | 33.896 | 22.286 | 73.305 | 1.00 | 45.44 | 8 |
| ATOM | 1976 | N | GLU A 249 | 34.788 | 20.982 | 71.710 | 1.00 | 42.38 | 7 |
| ATOM | 1977 | CA | GLU A 249 | 36.151 | 21.263 | 72.136 | 1.00 | 41.56 | 6 |
| ATOM | 1978 | CB | GLU A 249 | 37.148 | 20.275 | 71.528 | 1.00 | 42.06 | 6 |
| ATOM | 1979 | CG | GLU A 249 | 36.935 | 18.816 | 71.887 | 1.00 | 44.28 | 6 |
| ATOM | 1980 | CD | GLU A 249 | 38.015 | 17.908 | 71.295 | 1.00 | 44.79 | 6 |

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Figure 17-31

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1981 | OE1 | GLU | A | 249 | 38.208 | 17.938 | 70.054 | 1.00 | 42.47 | 8 |
| ATOM | 1982 | OE2 | GLU | A | 249 | 38.666 | 17.168 | 72.072 | 1.00 | 39.73 | 8 |
| ATOM | 1983 | C | GLU | A | 249 | 36.443 | 22.654 | 71.583 | 1.00 | 40.99 | 6 |
| ATOM | 1984 | O | GLU | A | 249 | 37.150 | 23.450 | 72.204 | 1.00 | 42.83 | 8 |
| ATOM | 1985 | N | VAL | A | 250 | 35.879 | 22.936 | 70.407 | 1.00 | 37.65 | 7 |
| ATOM | 1986 | CA | VAL | A | 250 | 36.059 | 24.221 | 69.728 | 1.00 | 34.87 | 6 |
| ATOM | 1987 | CB | VAL | A | 250 | 37.294 | 24.203 | 68.789 | 1.00 | 34.53 | 6 |
| ATOM | 1988 | CG1 | VAL | A | 250 | 37.129 | 23.113 | 67.728 | 1.00 | 32.76 | 6 |
| ATOM | 1989 | CG2 | VAL | A | 250 | 37.487 | 25.581 | 68.144 | 1.00 | 29.62 | 6 |
| ATOM | 1990 | C | VAL | A | 250 | 34.830 | 24.527 | 68.891 | 1.00 | 32.67 | 6 |
| ATOM | 1991 | O | VAL | A | 250 | 34.162 | 23.610 | 68.421 | 1.00 | 33.96 | 8 |
| ATOM | 1992 | N | TYR | A | 251 | 34.539 | 25.810 | 68.690 | 1.00 | 29.71 | 7 |
| ATOM | 1993 | CA | TYR | A | 251 | 33.368 | 26.183 | 67.916 | 1.00 | 27.07 | 6 |
| ATOM | 1994 | CB | TYR | A | 251 | 32.185 | 26.451 | 68.860 | 1.00 | 29.11 | 6 |
| ATOM | 1995 | CG | TYR | A | 251 | 32.080 | 27.872 | 69.406 | 1.00 | 31.46 | 6 |
| ATOM | 1996 | CD1 | TYR | A | 251 | 31.553 | 28.903 | 68.622 | 1.00 | 31.14 | 6 |
| ATOM | 1997 | CE1 | TYR | A | 251 | 31.439 | 30.196 | 69.106 | 1.00 | 31.66 | 6 |
| ATOM | 1998 | CD2 | TYR | A | 251 | 32.494 | 28.181 | 70.696 | 1.00 | 30.20 | 6 |
| ATOM | 1999 | CE2 | TYR | A | 251 | 32.384 | 29.477 | 71.193 | 1.00 | 33.89 | 6 |
| ATOM | 2000 | CZ | TYR | A | 251 | 31.854 | 30.482 | 70.391 | 1.00 | 34.75 | 6 |
| ATOM | 2001 | OH | TYR | A | 251 | 31.743 | 31.773 | 70.867 | 1.00 | 33.52 | 8 |
| ATOM | 2002 | C | TYR | A | 251 | 33.570 | 27.384 | 66.992 | 1.00 | 27.48 | 6 |
| ATOM | 2003 | O | TYR | A | 251 | 34.167 | 28.402 | 67.366 | 1.00 | 24.78 | 8 |
| ATOM | 2004 | N | LEU | A | 252 | 33.063 | 27.254 | 65.773 | 1.00 | 24.80 | 7 |
| ATOM | 2005 | CA | LEU | A | 252 | 33.150 | 28.332 | 64.815 | 1.00 | 23.40 | 6 |
| ATOM | 2006 | CB | LEU | A | 252 | 33.631 | 27.810 | 63.451 | 1.00 | 21.32 | 6 |
| ATOM | 2007 | CG | LEU | A | 252 | 35.126 | 27.456 | 63.385 | 1.00 | 21.84 | 6 |
| ATOM | 2008 | CD1 | LEU | A | 252 | 35.457 | 26.373 | 64.395 | 1.00 | 22.51 | 6 |
| ATOM | 2009 | CD2 | LEU | A | 252 | 35.499 | 26.999 | 61.986 | 1.00 | 22.07 | 6 |
| ATOM | 2010 | C | LEU | A | 252 | 31.762 | 28.959 | 64.729 | 1.00 | 22.56 | 6 |
| ATOM | 2011 | O | LEU | A | 252 | 30.750 | 28.266 | 64.856 | 1.00 | 21.99 | 8 |
| ATOM | 2012 | N | LEU | A | 253 | 31.734 | 30.277 | 64.554 | 1.00 | 21.01 | 7 |
| ATOM | 2013 | CA | LEU | A | 253 | 30.498 | 31.047 | 64.461 | 1.00 | 18.89 | 6 |
| ATOM | 2014 | CB | LEU | A | 253 | 30.352 | 31.944 | 65.695 | 1.00 | 20.05 | 6 |
| ATOM | 2015 | CG | LEU | A | 253 | 29.198 | 32.942 | 65.842 | 1.00 | 21.61 | 6 |
| ATOM | 2016 | CD1 | LEU | A | 253 | 27.849 | 32.220 | 65.860 | 1.00 | 22.23 | 6 |
| ATOM | 2017 | CD2 | LEU | A | 253 | 29.395 | 33.716 | 67.145 | 1.00 | 22.90 | 6 |
| ATOM | 2018 | C | LEU | A | 253 | 30.539 | 31.901 | 63.198 | 1.00 | 20.05 | 6 |
| ATOM | 2019 | O | LEU | A | 253 | 31.466 | 32.691 | 62.987 | 1.00 | 18.17 | 8 |
| ATOM | 2020 | N | GLN | A | 254 | 29.544 | 31.720 | 62.340 | 1.00 | 19.40 | 7 |
| ATOM | 2021 | CA | GLN | A | 254 | 29.488 | 32.490 | 61.115 | 1.00 | 18.17 | 6 |
| ATOM | 2022 | CB | GLN | A | 254 | 29.017 | 31.592 | 59.969 | 1.00 | 9.67 | 6 |
| ATOM | 2023 | CG | GLN | A | 254 | 27.584 | 31.713 | 59.601 | 1.00 | 18.43 | 6 |
| ATOM | 2024 | CD | GLN | A | 254 | 27.368 | 32.766 | 58.549 | 1.00 | 19.97 | 6 |
| ATOM | 2025 | OE1 | GLN | A | 254 | 27.917 | 32.677 | 57.450 | 1.00 | 22.54 | 8 |
| ATOM | 2026 | NE2 | GLN | A | 254 | 26.564 | 33.769 | 58.869 | 1.00 | 22.89 | 7 |
| ATOM | 2027 | C | GLN | A | 254 | 28.520 | 33.634 | 61.444 | 1.00 | 19.75 | 6 |
| ATOM | 2028 | O | GLN | A | 254 | 27.470 | 33.415 | 62.060 | 1.00 | 18.77 | 8 |
| ATOM | 2029 | N | LEU | A | 255 | 28.905 | 34.854 | 61.067 | 1.00 | 23.02 | 7 |
| ATOM | 2030 | CA | LEU | A | 255 | 28.132 | 36.052 | 61.369 | 1.00 | 23.77 | 6 |
| ATOM | 2031 | CB | LEU | A | 255 | 28.963 | 36.993 | 62.242 | 1.00 | 26.84 | 6 |
| ATOM | 2032 | CG | LEU | A | 255 | 29.226 | 36.556 | 63.684 | 1.00 | 29.34 | 6 |
| ATOM | 2033 | CD1 | LEU | A | 255 | 30.196 | 37.520 | 64.331 | 1.00 | 30.65 | 6 |
| ATOM | 2034 | CD2 | LEU | A | 255 | 27.902 | 36.506 | 64.456 | 1.00 | 28.42 | 6 |
| ATOM | 2035 | C | LEU | A | 255 | 27.605 | 36.842 | 60.197 | 1.00 | 24.84 | 6 |
| ATOM | 2036 | O | LEU | A | 255 | 27.774 | 38.066 | 60.149 | 1.00 | 24.94 | 8 |
| ATOM | 2037 | N | GLY | A | 256 | 26.969 | 36.158 | 59.254 | 1.00 | 25.07 | 7 |
| ATOM | 2038 | CA | GLY | A | 256 | 26.408 | 36.858 | 58.117 | 1.00 | 26.11 | 6 |
| ATOM | 2039 | C | GLY | A | 256 | 25.506 | 37.956 | 58.644 | 1.00 | 27.11 | 6 |
| ATOM | 2040 | O | GLY | A | 256 | 24.742 | 37.734 | 59.584 | 1.00 | 25.67 | 8 |
| ATOM | 2041 | N | THR | A | 257 | 25.599 | 39.150 | 58.072 | 1.00 | 27.85 | 7 |
| ATOM | 2042 | CA | THR | A | 257 | 24.757 | 40.244 | 58.536 | 1.00 | 29.28 | 6 |
| ATOM | 2043 | CB | THR | A | 257 | 25.517 | 41.597 | 58.545 | 1.00 | 27.98 | 6 |
| ATOM | 2044 | OG1 | THR | A | 257 | 26.002 | 41.895 | 57.232 | 1.00 | 31.91 | 8 |
| ATOM | 2045 | CG2 | THR | A | 257 | 26.686 | 41.541 | 59.510 | 1.00 | 26.45 | 6 |
| ATOM | 2046 | C | THR | A | 257 | 23.477 | 40.392 | 57.722 | 1.00 | 28.39 | 6 |

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Figure 17-32

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2047 | O | THR | A | 257 | 22.747 | 41.370 | 57.879 | 1.00 | 29.49 | 8 |
| ATOM | 2048 | N | ASP | A | 258 | 23.192 | 39.414 | 56.867 | 1.00 | 29.13 | 7 |
| ATOM | 2049 | CA | ASP | A | 258 | 21.977 | 39.471 | 56.065 | 1.00 | 30.49 | 6 |
| ATOM | 2050 | CB | ASP | A | 258 | 22.004 | 38.432 | 54.933 | 1.00 | 28.22 | 6 |
| ATOM | 2051 | CG | ASP | A | 258 | 22.337 | 37.033 | 55.416 | 1.00 | 29.39 | 6 |
| ATOM | 2052 | OD1 | ASP | A | 258 | 21.893 | 36.653 | 56.520 | 1.00 | 30.16 | 8 |
| ATOM | 2053 | OD2 | ASP | A | 258 | 23.019 | 36.292 | 54.667 | 1.00 | 29.97 | 8 |
| ATOM | 2054 | C | ASP | A | 258 | 20.646 | 39.355 | 56.826 | 1.00 | 30.50 | 6 |
| ATOM | 2055 | O | ASP | A | 258 | 19.601 | 39.622 | 56.248 | 1.00 | 32.87 | 8 |
| ATOM | 2056 | N | PRO | A | 259 | 20.650 | 38.912 | 58.101 | 1.00 | 30.76 | 7 |
| ATOM | 2057 | CD | PRO | A | 259 | 21.711 | 38.338 | 58.952 | 1.00 | 33.56 | 6 |
| ATOM | 2058 | CA | PRO | A | 259 | 19.366 | 38.821 | 58.806 | 1.00 | 31.73 | 6 |
| ATOM | 2059 | CB | PRO | A | 259 | 19.705 | 37.912 | 59.987 | 1.00 | 31.87 | 6 |
| ATOM | 2060 | CG | PRO | A | 259 | 21.067 | 38.373 | 60.333 | 1.00 | 31.73 | 6 |
| ATOM | 2061 | C | PRO | A | 259 | 18.817 | 40.184 | 59.260 | 1.00 | 30.86 | 6 |
| ATOM | 2062 | O | PRO | A | 259 | 17.736 | 40.270 | 59.845 | 1.00 | 29.78 | 8 |
| ATOM | 2063 | N | LEU | A | 260 | 19.565 | 41.245 | 58.980 | 1.00 | 29.58 | 7 |
| ATOM | 2064 | CA | LEU | A | 260 | 19.161 | 42.592 | 59.375 | 1.00 | 29.15 | 6 |
| ATOM | 2065 | CB | LEU | A | 260 | 20.367 | 43.542 | 59.275 | 1.00 | 27.14 | 6 |
| ATOM | 2066 | CG | LEU | A | 260 | 21.543 | 43.286 | 60.234 | 1.00 | 22.17 | 6 |
| ATOM | 2067 | CD1 | LEU | A | 260 | 22.794 | 43.919 | 59.684 | 1.00 | 15.79 | 6 |
| ATOM | 2068 | CD2 | LEU | A | 260 | 21.211 | 43.793 | 61.633 | 1.00 | 16.25 | 6 |
| ATOM | 2069 | C | LEU | A | 260 | 17.992 | 43.165 | 58.576 | 1.00 | 28.09 | 6 |
| ATOM | 2070 | O | LEU | A | 260 | 17.787 | 42.834 | 57.410 | 1.00 | 29.61 | 8 |
| ATOM | 2071 | N | LEU | A | 261 | 17.237 | 44.044 | 59.223 | 1.00 | 29.29 | 7 |
| ATOM | 2072 | CA | LEU | A | 261 | 16.097 | 44.693 | 58.596 | 1.00 | 29.71 | 6 |
| ATOM | 2073 | CB | LEU | A | 261 | 15.540 | 45.788 | 59.513 | 1.00 | 29.62 | 6 |
| ATOM | 2074 | CG | LEU | A | 261 | 14.406 | 46.664 | 58.950 | 1.00 | 28.14 | 6 |
| ATOM | 2075 | CD1 | LEU | A | 261 | 13.144 | 45.819 | 58.803 | 1.00 | 24.82 | 6 |
| ATOM | 2076 | CD2 | LEU | A | 261 | 14.139 | 47.859 | 59.882 | 1.00 | 25.45 | 6 |
| ATOM | 2077 | C | LEU | A | 261 | 16.461 | 45.322 | 57.259 | 1.00 | 29.50 | 6 |
| ATOM | 2078 | O | LEU | A | 261 | 15.717 | 45.198 | 56.295 | 1.00 | 31.67 | 8 |
| ATOM | 2079 | N | GLU | A | 262 | 17.603 | 45.998 | 57.201 | 1.00 | 31.54 | 7 |
| ATOM | 2080 | CA | GLU | A | 262 | 18.015 | 46.664 | 55.973 | 1.00 | 31.93 | 6 |
| ATOM | 2081 | CB | GLU | A | 262 | 19.049 | 47.758 | 56.279 | 1.00 | 29.34 | 6 |
| ATOM | 2082 | CG | GLU | A | 262 | 18.496 | 48.931 | 57.086 | 1.00 | 28.52 | 6 |
| ATOM | 2083 | CD | GLU | A | 262 | 18.449 | 48.687 | 58.589 | 1.00 | 29.76 | 6 |
| ATOM | 2084 | OE1 | GLU | A | 262 | 18.175 | 47.548 | 59.029 | 1.00 | 30.12 | 8 |
| ATOM | 2085 | OE2 | GLU | A | 262 | 18.661 | 49.661 | 59.338 | 1.00 | 27.69 | 8 |
| ATOM | 2086 | C | GLU | A | 262 | 18.526 | 45.754 | 54.857 | 1.00 | 34.29 | 6 |
| ATOM | 2087 | O | GLU | A | 262 | 18.690 | 46.199 | 53.722 | 1.00 | 35.20 | 8 |
| ATOM | 2088 | N | ASP | A | 263 | 18.778 | 44.486 | 55.158 | 1.00 | 36.55 | 7 |
| ATOM | 2089 | CA | ASP | A | 263 | 19.245 | 43.582 | 54.117 | 1.00 | 39.50 | 6 |
| ATOM | 2090 | CB | ASP | A | 263 | 20.354 | 42.672 | 54.641 | 1.00 | 38.42 | 6 |
| ATOM | 2091 | CG | ASP | A | 263 | 20.982 | 41.847 | 53.538 | 1.00 | 39.33 | 6 |
| ATOM | 2092 | OD1 | ASP | A | 263 | 22.064 | 41.263 | 53.762 | 1.00 | 38.86 | 8 |
| ATOM | 2093 | OD2 | ASP | A | 263 | 20.384 | 41.779 | 52.443 | 1.00 | 39.50 | 8 |
| ATOM | 2094 | C | ASP | A | 263 | 18.046 | 42.775 | 53.634 | 1.00 | 42.83 | 6 |
| ATOM | 2095 | O | ASP | A | 263 | 17.474 | 41.966 | 54.381 | 1.00 | 44.22 | 8 |
| ATOM | 2096 | N | TYR | A | 264 | 17.673 | 43.002 | 52.377 | 1.00 | 44.14 | 7 |
| ATOM | 2097 | CA | TYR | A | 264 | 16.508 | 42.357 | 51.796 | 1.00 | 46.67 | 6 |
| ATOM | 2098 | CB | TYR | A | 264 | 16.031 | 43.149 | 50.568 | 1.00 | 54.61 | 6 |
| ATOM | 2099 | CG | TYR | A | 264 | 16.824 | 42.939 | 49.294 | 1.00 | 63.02 | 6 |
| ATOM | 2100 | CD1 | TYR | A | 264 | 16.510 | 41.897 | 48.412 | 1.00 | 65.73 | 6 |
| ATOM | 2101 | CE1 | TYR | A | 264 | 17.230 | 41.709 | 47.226 | 1.00 | 68.35 | 6 |
| ATOM | 2102 | CD2 | TYR | A | 264 | 17.882 | 43.786 | 48.962 | 1.00 | 66.23 | 6 |
| ATOM | 2103 | CE2 | TYR | A | 264 | 18.611 | 43.606 | 47.780 | 1.00 | 68.63 | 6 |
| ATOM | 2104 | CZ | TYR | A | 264 | 18.279 | 42.570 | 46.918 | 1.00 | 69.08 | 6 |
| ATOM | 2105 | OH | TYR | A | 264 | 18.989 | 42.411 | 45.746 | 1.00 | 69.01 | 8 |
| ATOM | 2106 | C | TYR | A | 264 | 16.665 | 40.888 | 51.451 | 1.00 | 43.89 | 6 |
| ATOM | 2107 | O | TYR | A | 264 | 15.663 | 40.185 | 51.293 | 1.00 | 44.80 | 8 |
| ATOM | 2108 | N | LEU | A | 265 | 17.897 | 40.400 | 51.333 | 1.00 | 40.37 | 7 |
| ATOM | 2109 | CA | LEU | A | 265 | 18.051 | 38.984 | 51.016 | 1.00 | 38.06 | 6 |
| ATOM | 2110 | CB | LEU | A | 265 | 19.474 | 38.646 | 50.538 | 1.00 | 33.48 | 6 |
| ATOM | 2111 | CG | LEU | A | 265 | 19.905 | 39.211 | 49.172 | 1.00 | 32.43 | 6 |
| ATOM | 2112 | CD1 | LEU | A | 265 | 21.176 | 38.535 | 48.703 | 1.00 | 26.97 | 6 |

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Figure 17-33

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2113 | CD2 | LEU | A | 265 | 18.828 | 38.954 | 48.141 | 1.00 | 34.41 | 6 |
| ATOM | 2114 | C | LEU | A | 265 | 17.665 | 38.131 | 52.219 | 1.00 | 37.41 | 6 |
| ATOM | 2115 | O | LEU | A | 265 | 18.125 | 37.000 | 52.370 | 1.00 | 37.96 | 8 |
| ATOM | 2116 | N | SER | A | 266 | 16.804 | 38.694 | 53.066 | 1.00 | 36.21 | 7 |
| ATOM | 2117 | CA | SER | A | 266 | 16.294 | 38.013 | 54.253 | 1.00 | 36.46 | 6 |
| ATOM | 2118 | CB | SER | A | 266 | 17.263 | 38.136 | 55.427 | 1.00 | 37.22 | 6 |
| ATOM | 2119 | OG | SER | A | 266 | 17.190 | 39.440 | 55.991 | 1.00 | 37.41 | 8 |
| ATOM | 2120 | C | SER | A | 266 | 14.997 | 38.705 | 54.653 | 1.00 | 35.55 | 6 |
| ATOM | 2121 | O | SER | A | 266 | 14.889 | 39.927 | 54.568 | 1.00 | 37.09 | 8 |
| ATOM | 2122 | N | LYS | A | 267 | 14.018 | 37.928 | 55.093 | 1.00 | 34.33 | 7 |
| ATOM | 2123 | CA | LYS | A | 267 | 12.750 | 38.493 | 55.532 | 1.00 | 36.13 | 6 |
| ATOM | 2124 | CB | LYS | A | 267 | 11.596 | 37.548 | 55.183 | 1.00 | 36.11 | 6 |
| ATOM | 2125 | CG | LYS | A | 267 | 11.503 | 37.222 | 53.705 | 1.00 | 36.79 | 6 |
| ATOM | 2126 | CD | LYS | A | 267 | 11.453 | 38.487 | 52.869 | 1.00 | 38.55 | 6 |
| ATOM | 2127 | CE | LYS | A | 267 | 11.369 | 38.170 | 51.389 | 1.00 | 41.60 | 6 |
| ATOM | 2128 | NZ | LYS | A | 267 | 11.503 | 39.413 | 50.569 | 1.00 | 42.07 | 7 |
| ATOM | 2129 | C | LYS | A | 267 | 12.791 | 38.738 | 57.043 | 1.00 | 34.90 | 6 |
| ATOM | 2130 | O | LYS | A | 267 | 11.758 | 38.867 | 57.694 | 1.00 | 37.18 | 8 |
| ATOM | 2131 | N | PHE | A | 268 | 13.998 | 38.775 | 57.595 | 1.00 | 32.82 | 7 |
| ATOM | 2132 | CA | PHE | A | 268 | 14.192 | 39.021 | 59.016 | 1.00 | 31.50 | 6 |
| ATOM | 2133 | CB | PHE | A | 268 | 15.477 | 38.337 | 59.495 | 1.00 | 34.05 | 6 |
| ATOM | 2134 | CG | PHE | A | 268 | 15.379 | 36.839 | 59.604 | 1.00 | 34.54 | 6 |
| ATOM | 2135 | CD1 | PHE | A | 268 | 16.506 | 36.087 | 59.940 | 1.00 | 35.04 | 6 |
| ATOM | 2136 | CD2 | PHE | A | 268 | 14.161 | 36.178 | 59.429 | 1.00 | 34.57 | 6 |
| ATOM | 2137 | CE1 | PHE | A | 268 | 16.423 | 34.691 | 60.108 | 1.00 | 35.44 | 6 |
| ATOM | 2138 | CE2 | PHE | A | 268 | 14.066 | 34.784 | 59.594 | 1.00 | 36.00 | 6 |
| ATOM | 2139 | CZ | PHE | A | 268 | 15.201 | 34.040 | 59.936 | 1.00 | 34.68 | 6 |
| ATOM | 2140 | C | PHE | A | 268 | 14.319 | 40.530 | 59.190 | 1.00 | 30.94 | 6 |
| ATOM | 2141 | O | PHE | A | 268 | 14.983 | 41.192 | 58.394 | 1.00 | 30.27 | 8 |
| ATOM | 2142 | N | ASN | A | 269 | 13.693 | 41.081 | 60.222 | 1.00 | 32.53 | 7 |
| ATOM | 2143 | CA | ASN | A | 269 | 13.760 | 42.527 | 60.448 | 1.00 | 35.83 | 6 |
| ATOM | 2144 | CB | ASN | A | 269 | 12.344 | 43.115 | 60.570 | 1.00 | 37.23 | 6 |
| ATOM | 2145 | CG | ASN | A | 269 | 11.478 | 42.809 | 59.360 | 1.00 | 40.75 | 6 |
| ATOM | 2146 | OD1 | ASN | A | 269 | 11.830 | 43.148 | 58.227 | 1.00 | 43.88 | 8 |
| ATOM | 2147 | ND2 | ASN | A | 269 | 10.335 | 42.165 | 59.594 | 1.00 | 39.61 | 7 |
| ATOM | 2148 | C | ASN | A | 269 | 14.553 | 42.854 | 61.710 | 1.00 | 35.45 | 6 |
| ATOM | 2149 | O | ASN | A | 269 | 14.095 | 43.621 | 62.560 | 1.00 | 41.47 | 8 |
| ATOM | 2150 | N | LEU | A | 270 | 15.747 | 42.285 | 61.827 | 1.00 | 33.27 | 7 |
| ATOM | 2151 | CA | LEU | A | 270 | 16.571 | 42.510 | 63.004 | 1.00 | 30.68 | 6 |
| ATOM | 2152 | CB | LEU | A | 270 | 17.638 | 41.431 | 63.114 | 1.00 | 27.41 | 6 |
| ATOM | 2153 | CG | LEU | A | 270 | 17.140 | 40.002 | 62.988 | 1.00 | 23.76 | 6 |
| ATOM | 2154 | CD1 | LEU | A | 270 | 18.222 | 39.106 | 63.543 | 1.00 | 27.14 | 6 |
| ATOM | 2155 | CD2 | LEU | A | 270 | 15.855 | 39.801 | 63.772 | 1.00 | 28.00 | 6 |
| ATOM | 2156 | C | LEU | A | 270 | 17.258 | 43.856 | 63.033 | 1.00 | 32.30 | 6 |
| ATOM | 2157 | O | LEU | A | 270 | 17.347 | 44.554 | 62.017 | 1.00 | 36.27 | 8 |
| ATOM | 2158 | N | SER | A | 271 | 17.749 | 44.207 | 64.216 | 1.00 | 30.33 | 7 |
| ATOM | 2159 | CA | SER | A | 271 | 18.465 | 45.457 | 64.424 | 1.00 | 30.79 | 6 |
| ATOM | 2160 | CB | SER | A | 271 | 17.816 | 46.249 | 65.562 | 1.00 | 29.53 | 6 |
| ATOM | 2161 | OG | SER | A | 271 | 17.712 | 45.471 | 66.739 | 1.00 | 30.43 | 8 |
| ATOM | 2162 | C | SER | A | 271 | 19.911 | 45.109 | 64.768 | 1.00 | 33.09 | 6 |
| ATOM | 2163 | O | SER | A | 271 | 20.194 | 43.972 | 65.172 | 1.00 | 29.64 | 8 |
| ATOM | 2164 | N | ASN | A | 272 | 20.821 | 46.069 | 64.586 | 1.00 | 32.36 | 7 |
| ATOM | 2165 | CA | ASN | A | 272 | 22.234 | 45.846 | 64.896 | 1.00 | 31.65 | 6 |
| ATOM | 2166 | CB | ASN | A | 272 | 23.036 | 47.141 | 64.771 | 1.00 | 33.76 | 6 |
| ATOM | 2167 | CG | ASN | A | 272 | 23.101 | 47.658 | 63.361 | 1.00 | 37.76 | 6 |
| ATOM | 2168 | OD1 | ASN | A | 272 | 23.719 | 48.686 | 63.100 | 1.00 | 36.12 | 8 |
| ATOM | 2169 | ND2 | ASN | A | 272 | 22.460 | 46.952 | 62.437 | 1.00 | 44.79 | 7 |
| ATOM | 2170 | C | ASN | A | 272 | 22.369 | 45.333 | 66.321 | 1.00 | 32.61 | 6 |
| ATOM | 2171 | O | ASN | A | 272 | 22.970 | 44.283 | 66.565 | 1.00 | 27.95 | 8 |
| ATOM | 2172 | N | VAL | A | 273 | 21.803 | 46.091 | 67.257 | 1.00 | 33.22 | 7 |
| ATOM | 2173 | CA | VAL | A | 273 | 21.839 | 45.741 | 68.668 | 1.00 | 35.52 | 6 |
| ATOM | 2174 | CB | VAL | A | 273 | 20.928 | 46.660 | 69.481 | 1.00 | 37.80 | 6 |
| ATOM | 2175 | CG1 | VAL | A | 273 | 20.987 | 46.276 | 70.964 | 1.00 | 39.00 | 6 |
| ATOM | 2176 | CG2 | VAL | A | 273 | 21.356 | 48.112 | 69.275 | 1.00 | 38.88 | 6 |
| ATOM | 2177 | C | VAL | A | 273 | 21.416 | 44.300 | 68.908 | 1.00 | 34.26 | 6 |
| ATOM | 2178 | O | VAL | A | 273 | 22.060 | 43.580 | 69.679 | 1.00 | 35.96 | 8 |

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Figure 17-34

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATCM | 2179 | N | ALA | A | 274 | 20.328 | 43.889 | 68.262 | 1.00 | 32.36 | 7 |
| ATCM | 2180 | CA | ALA | A | 274 | 19.834 | 42.521 | 68.385 | 1.00 | 31.09 | 6 |
| ATCM | 2181 | CB | ALA | A | 274 | 18.574 | 42.356 | 67.578 | 1.00 | 28.88 | 6 |
| ATCM | 2182 | C | ALA | A | 274 | 20.923 | 41.588 | 67.861 | 1.00 | 31.74 | 6 |
| ATCM | 2183 | O | ALA | A | 274 | 21.323 | 40.634 | 68.533 | 1.00 | 31.54 | 8 |
| ATCM | 2184 | N | PHE | A | 275 | 21.401 | 41.879 | 66.655 | 1.00 | 30.05 | 7 |
| ATCM | 2185 | CA | PHE | A | 275 | 22.467 | 41.102 | 66.036 | 1.00 | 31.30 | 6 |
| ATCM | 2186 | CB | PHE | A | 275 | 22.932 | 41.810 | 64.751 | 1.00 | 31.54 | 6 |
| ATCM | 2187 | CG | PHE | A | 275 | 23.938 | 41.029 | 63.941 | 1.00 | 31.76 | 6 |
| ATCM | 2188 | CD1 | PHE | A | 275 | 23.597 | 39.809 | 63.365 | 1.00 | 32.40 | 6 |
| ATCM | 2189 | CD2 | PHE | A | 275 | 25.219 | 41.529 | 63.729 | 1.00 | 34.04 | 6 |
| ATCM | 2190 | CE1 | PHE | A | 275 | 24.513 | 39.100 | 62.586 | 1.00 | 32.27 | 6 |
| ATCM | 2191 | CE2 | PHE | A | 275 | 26.149 | 40.828 | 62.950 | 1.00 | 33.90 | 6 |
| ATCM | 2192 | CZ | PHE | A | 275 | 25.793 | 39.613 | 62.378 | 1.00 | 34.50 | 6 |
| ATCM | 2193 | C | PHE | A | 275 | 23.632 | 40.999 | 67.040 | 1.00 | 29.98 | 6 |
| ATCM | 2194 | O | PHE | A | 275 | 24.252 | 39.950 | 67.200 | 1.00 | 29.41 | 8 |
| ATCM | 2195 | N | LEU | A | 276 | 23.908 | 42.099 | 67.726 | 1.00 | 31.22 | 7 |
| ATCM | 2196 | CA | LEU | A | 276 | 24.988 | 42.144 | 68.698 | 1.00 | 32.29 | 6 |
| ATCM | 2197 | CB | LEU | A | 276 | 25.221 | 43.594 | 69.141 | 1.00 | 33.44 | 6 |
| ATCM | 2198 | CG | LEU | A | 276 | 26.415 | 43.908 | 70.050 | 1.00 | 36.01 | 6 |
| ATCM | 2199 | CD1 | LEU | A | 276 | 26.683 | 45.391 | 70.025 | 1.00 | 35.02 | 6 |
| ATCM | 2200 | CD2 | LEU | A | 276 | 26.147 | 43.433 | 71.467 | 1.00 | 39.09 | 6 |
| ATCM | 2201 | C | LEU | A | 276 | 24.682 | 41.244 | 69.894 | 1.00 | 32.79 | 6 |
| ATCM | 2202 | O | LEU | A | 276 | 25.560 | 40.530 | 70.371 | 1.00 | 30.74 | 8 |
| ATCM | 2203 | N | LYS | A | 277 | 23.445 | 41.273 | 70.384 | 1.00 | 33.95 | 7 |
| ATCM | 2204 | CA | LYS | A | 277 | 23.086 | 40.413 | 71.505 | 1.00 | 36.56 | 6 |
| ATCM | 2205 | CB | LYS | A | 277 | 21.623 | 40.588 | 71.902 | 1.00 | 35.76 | 6 |
| ATCM | 2206 | CG | LYS | A | 277 | 21.343 | 41.842 | 72.687 | 1.00 | 42.31 | 6 |
| ATCM | 2207 | CD | LYS | A | 277 | 20.743 | 41.508 | 74.049 | 1.00 | 45.72 | 6 |
| ATCM | 2208 | CE | LYS | A | 277 | 21.665 | 40.601 | 74.865 | 1.00 | 47.87 | 6 |
| ATCM | 2209 | NZ | LYS | A | 277 | 21.140 | 40.378 | 76.244 | 1.00 | 44.36 | 7 |
| ATCM | 2210 | C | LYS | A | 277 | 23.302 | 38.974 | 71.092 | 1.00 | 37.98 | 6 |
| ATCM | 2211 | O | LYS | A | 277 | 23.875 | 38.179 | 71.845 | 1.00 | 37.54 | 8 |
| ATCM | 2212 | N | ALA | A | 278 | 22.832 | 38.654 | 69.886 | 1.00 | 37.17 | 7 |
| ATCM | 2213 | CA | ALA | A | 278 | 22.952 | 37.311 | 69.323 | 1.00 | 34.51 | 6 |
| ATCM | 2214 | CB | ALA | A | 278 | 22.638 | 37.341 | 67.820 | 1.00 | 35.38 | 6 |
| ATCM | 2215 | C | ALA | A | 278 | 24.368 | 36.831 | 69.550 | 1.00 | 30.63 | 6 |
| ATCM | 2216 | O | ALA | A | 278 | 24.605 | 35.790 | 70.167 | 1.00 | 27.62 | 8 |
| ATCM | 2217 | N | PHE | A | 279 | 25.303 | 37.624 | 69.049 | 1.00 | 29.24 | 7 |
| ATCM | 2218 | CA | PHE | A | 279 | 26.722 | 37.347 | 69.167 | 1.00 | 31.48 | 6 |
| ATCM | 2219 | CB | PHE | A | 279 | 27.490 | 38.558 | 68.645 | 1.00 | 33.25 | 6 |
| ATCM | 2220 | CG | PHE | A | 279 | 28.974 | 38.396 | 68.663 | 1.00 | 39.28 | 6 |
| ATCM | 2221 | CD1 | PHE | A | 279 | 29.578 | 37.337 | 68.000 | 1.00 | 41.15 | 6 |
| ATCM | 2222 | CD2 | PHE | A | 279 | 29.776 | 39.328 | 69.315 | 1.00 | 40.66 | 6 |
| ATCM | 2223 | CE1 | PHE | A | 279 | 30.960 | 37.209 | 67.987 | 1.00 | 44.22 | 6 |
| ATCM | 2224 | CE2 | PHE | A | 279 | 31.153 | 39.213 | 69.378 | 1.00 | 41.38 | 6 |
| ATCM | 2225 | CZ | PHE | A | 279 | 31.750 | 38.152 | 68.614 | 1.00 | 44.52 | 6 |
| ATCM | 2226 | C | PHE | A | 279 | 27.116 | 37.043 | 70.611 | 1.00 | 31.81 | 6 |
| ATCM | 2227 | O | PHE | A | 279 | 27.627 | 35.953 | 70.935 | 1.00 | 27.51 | 8 |
| ATCM | 2228 | N | ASN | A | 280 | 26.860 | 38.005 | 71.503 | 1.00 | 29.32 | 7 |
| ATCM | 2229 | CA | ASN | A | 280 | 27.192 | 37.851 | 72.907 | 1.00 | 29.26 | 6 |
| ATCM | 2230 | CB | ASN | A | 280 | 26.927 | 39.153 | 73.660 | 1.00 | 30.39 | 6 |
| ATCM | 2231 | CG | ASN | A | 280 | 27.907 | 40.245 | 73.278 | 1.00 | 30.68 | 6 |
| ATCM | 2232 | OD1 | ASN | A | 280 | 29.117 | 40.030 | 73.303 | 1.00 | 33.34 | 8 |
| ATCM | 2233 | ND2 | ASN | A | 280 | 27.395 | 41.419 | 72.931 | 1.00 | 27.00 | 7 |
| ATCM | 2234 | C | ASN | A | 280 | 26.524 | 36.680 | 73.616 | 1.00 | 30.01 | 6 |
| ATCM | 2235 | O | ASN | A | 280 | 27.167 | 36.004 | 74.419 | 1.00 | 29.58 | 8 |
| ATCM | 2236 | N | ILE | A | 281 | 25.252 | 36.423 | 73.335 | 1.00 | 30.46 | 7 |
| ATCM | 2237 | CA | ILE | A | 281 | 24.594 | 35.291 | 73.983 | 1.00 | 33.71 | 6 |
| ATCM | 2238 | CB | ILE | A | 281 | 23.107 | 35.161 | 73.569 | 1.00 | 36.14 | 6 |
| ATCM | 2239 | CG2 | ILE | A | 281 | 22.541 | 33.820 | 74.032 | 1.00 | 36.18 | 6 |
| ATCM | 2240 | CG1 | ILE | A | 281 | 22.298 | 36.307 | 74.177 | 1.00 | 33.52 | 6 |
| ATCM | 2241 | CD1 | ILE | A | 281 | 20.835 | 36.243 | 73.834 | 1.00 | 37.16 | 6 |
| ATCM | 2242 | C | ILE | A | 281 | 25.330 | 34.006 | 73.631 | 1.00 | 34.06 | 6 |
| ATCM | 2243 | O | ILE | A | 281 | 25.385 | 33.071 | 74.437 | 1.00 | 31.94 | 8 |
| ATCM | 2244 | N | VAL | A | 282 | 25.896 | 33.960 | 72.427 | 1.00 | 35.31 | 7 |

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Figure 17-35

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 2245 | CA | VAL A 282 | 26.654 | 32.785 | 72.005 | 1.00 | 36.45 | 6 |
| ATOM | 2246 | CB | VAL A 282 | 27.084 | 32.871 | 70.524 | 1.00 | 35.62 | 6 |
| ATOM | 2247 | CG1 | VAL A 282 | 27.829 | 31.604 | 70.126 | 1.00 | 31.20 | 6 |
| ATOM | 2248 | CG2 | VAL A 282 | 25.880 | 33.080 | 69.646 | 1.00 | 34.51 | 6 |
| ATOM | 2249 | C | VAL A 282 | 27.919 | 32.723 | 72.857 | 1.00 | 37.80 | 6 |
| ATOM | 2250 | O | VAL A 282 | 28.182 | 31.722 | 73.532 | 1.00 | 36.12 | 8 |
| ATOM | 2251 | N | ARG A 283 | 28.693 | 33.808 | 72.821 | 1.00 | 38.45 | 7 |
| ATOM | 2252 | CA | ARG A 283 | 29.929 | 33.884 | 73.567 | 1.00 | 40.06 | 6 |
| ATOM | 2253 | CB | ARG A 283 | 30.551 | 35.272 | 73.449 | 1.00 | 39.38 | 6 |
| ATOM | 2254 | CG | ARG A 283 | 30.974 | 35.625 | 72.027 | 1.00 | 41.90 | 6 |
| ATOM | 2255 | CD | ARG A 283 | 31.492 | 37.048 | 71.968 | 1.00 | 41.36 | 6 |
| ATOM | 2256 | NE | ARG A 283 | 32.647 | 37.206 | 72.840 | 1.00 | 43.35 | 7 |
| ATOM | 2257 | CZ | ARG A 283 | 33.162 | 38.373 | 73.215 | 1.00 | 42.55 | 6 |
| ATOM | 2258 | NH1 | ARG A 283 | 32.628 | 39.516 | 72.797 | 1.00 | 39.95 | 7 |
| ATOM | 2259 | NH2 | ARG A 283 | 34.220 | 38.392 | 74.014 | 1.00 | 41.72 | 7 |
| ATOM | 2260 | C | ARG A 283 | 29.614 | 33.587 | 75.044 | 1.00 | 40.01 | 6 |
| ATOM | 2261 | O | ARG A 283 | 30.350 | 32.862 | 75.716 | 1.00 | 39.01 | 8 |
| ATOM | 2262 | N | GLU A 284 | 28.506 | 34.141 | 75.520 | 1.00 | 40.30 | 7 |
| ATOM | 2263 | CA | GLU A 284 | 28.084 | 33.923 | 76.894 | 1.00 | 43.19 | 6 |
| ATOM | 2264 | CB | GLU A 284 | 26.753 | 34.647 | 77.165 | 1.00 | 47.53 | 6 |
| ATOM | 2265 | CG | GLU A 284 | 26.875 | 36.176 | 77.090 | 1.00 | 56.10 | 6 |
| ATOM | 2266 | CD | GLU A 284 | 25.542 | 36.923 | 77.179 | 1.00 | 60.77 | 6 |
| ATOM | 2267 | OE1 | GLU A 284 | 24.659 | 36.682 | 76.329 | 1.00 | 61.41 | 8 |
| ATOM | 2268 | OE2 | GLU A 284 | 25.383 | 37.763 | 78.096 | 1.00 | 62.21 | 8 |
| ATOM | 2269 | C | GLU A 284 | 27.953 | 32.429 | 77.179 | 1.00 | 40.72 | 6 |
| ATOM | 2270 | O | GLU A 284 | 28.565 | 31.922 | 78.120 | 1.00 | 45.29 | 8 |
| ATOM | 2271 | N | VAL A 285 | 27.186 | 31.721 | 76.354 | 1.00 | 34.82 | 7 |
| ATOM | 2272 | CA | VAL A 285 | 26.975 | 30.288 | 76.551 | 1.00 | 30.84 | 6 |
| ATOM | 2273 | CB | VAL A 285 | 25.842 | 29.752 | 75.647 | 1.00 | 27.74 | 6 |
| ATOM | 2274 | CG1 | VAL A 285 | 25.698 | 28.253 | 75.831 | 1.00 | 22.95 | 6 |
| ATOM | 2275 | CG2 | VAL A 285 | 24.545 | 30.433 | 75.982 | 1.00 | 26.26 | 6 |
| ATOM | 2276 | C | VAL A 285 | 28.181 | 29.366 | 76.341 | 1.00 | 31.93 | 6 |
| ATOM | 2277 | O | VAL A 285 | 28.492 | 28.556 | 77.214 | 1.00 | 33.46 | 8 |
| ATOM | 2278 | N | PHE A 286 | 28.845 | 29.466 | 75.191 | 1.00 | 29.43 | 7 |
| ATOM | 2279 | CA | PHE A 286 | 29.973 | 28.586 | 74.907 | 1.00 | 24.26 | 6 |
| ATOM | 2280 | CB | PHE A 286 | 29.830 | 27.957 | 73.519 | 1.00 | 22.57 | 6 |
| ATOM | 2281 | CG | PHE A 286 | 28.607 | 27.095 | 73.345 | 1.00 | 23.46 | 6 |
| ATOM | 2282 | CD1 | PHE A 286 | 27.409 | 27.639 | 72.885 | 1.00 | 23.90 | 6 |
| ATOM | 2283 | CD2 | PHE A 286 | 28.664 | 25.718 | 73.608 | 1.00 | 21.95 | 6 |
| ATOM | 2284 | CE1 | PHE A 286 | 26.281 | 26.814 | 72.681 | 1.00 | 24.90 | 6 |
| ATOM | 2285 | CE2 | PHE A 286 | 27.547 | 24.892 | 73.411 | 1.00 | 18.06 | 6 |
| ATOM | 2286 | CZ | PHE A 286 | 26.357 | 25.437 | 72.945 | 1.00 | 20.23 | 6 |
| ATOM | 2287 | C | PHE A 286 | 31.368 | 29.200 | 74.991 | 1.00 | 25.14 | 6 |
| ATOM | 2288 | O | PHE A 286 | 32.338 | 28.566 | 74.560 | 1.00 | 23.16 | 8 |
| ATOM | 2289 | N | GLY A 287 | 31.480 | 30.416 | 75.525 | 1.00 | 25.51 | 7 |
| ATOM | 2290 | CA | GLY A 287 | 32.783 | 31.065 | 75.614 | 1.00 | 26.86 | 6 |
| ATOM | 2291 | C | GLY A 287 | 33.353 | 31.511 | 74.270 | 1.00 | 26.28 | 6 |
| ATOM | 2292 | O | GLY A 287 | 32.644 | 31.549 | 73.271 | 1.00 | 26.29 | 8 |
| ATOM | 2293 | N | GLU A 288 | 34.637 | 31.849 | 74.238 | 1.00 | 27.17 | 7 |
| ATOM | 2294 | CA | GLU A 288 | 35.274 | 32.291 | 72.996 | 1.00 | 33.20 | 6 |
| ATOM | 2295 | CB | GLU A 288 | 36.680 | 32.828 | 73.269 | 1.00 | 35.09 | 6 |
| ATOM | 2296 | CG | GLU A 288 | 36.726 | 34.104 | 74.083 | 1.00 | 41.67 | 6 |
| ATOM | 2297 | CD | GLU A 288 | 35.970 | 35.231 | 73.421 | 1.00 | 43.13 | 6 |
| ATOM | 2298 | OE1 | GLU A 288 | 36.221 | 35.493 | 72.228 | 1.00 | 45.39 | 8 |
| ATOM | 2299 | OE2 | GLU A 288 | 35.130 | 35.858 | 74.097 | 1.00 | 47.64 | 8 |
| ATOM | 2300 | C | GLU A 288 | 35.386 | 31.204 | 71.930 | 1.00 | 32.87 | 6 |
| ATOM | 2301 | O | GLU A 288 | 35.596 | 30.029 | 72.247 | 1.00 | 31.59 | 8 |
| ATOM | 2302 | N | GLY A 289 | 35.268 | 31.619 | 70.668 | 1.00 | 31.93 | 7 |
| ATOM | 2303 | CA | GLY A 289 | 35.373 | 30.698 | 69.545 | 1.00 | 29.58 | 6 |
| ATOM | 2304 | C | GLY A 289 | 35.948 | 31.372 | 68.307 | 1.00 | 27.42 | 5 |
| ATOM | 2305 | O | GLY A 289 | 36.556 | 32.437 | 68.398 | 1.00 | 26.27 | 8 |
| ATOM | 2306 | N | VAL A 290 | 35.764 | 30.758 | 67.143 | 1.00 | 27.64 | 7 |
| ATOM | 2307 | CA | VAL A 290 | 36.277 | 31.349 | 65.907 | 1.00 | 27.17 | 6 |
| ATOM | 2308 | CB | VAL A 290 | 37.014 | 30.301 | 65.037 | 1.00 | 25.25 | 6 |
| ATOM | 2309 | CG1 | VAL A 290 | 37.616 | 30.976 | 63.813 | 1.00 | 22.41 | 6 |
| ATOM | 2310 | CG2 | VAL A 290 | 38.100 | 29.632 | 65.852 | 1.00 | 17.33 | 6 |

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Figure 17-36

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2311 | C | VAL | A | 290 | 35.137 | 31.975 | 65.105 | 1.00 | 25.97 | 6 |
| ATOM | 2312 | O | VAL | A | 290 | 34.218 | 31.279 | 64.672 | 1.00 | 22.32 | 8 |
| ATOM | 2313 | N | TYR | A | 291 | 35.217 | 33.293 | 64.914 | 1.00 | 27.33 | 7 |
| ATOM | 2314 | CA | TYR | A | 291 | 34.188 | 34.052 | 64.203 | 1.00 | 26.69 | 6 |
| ATOM | 2315 | CB | TYR | A | 291 | 33.925 | 35.356 | 64.939 | 1.00 | 25.51 | 6 |
| ATOM | 2316 | CG | TYR | A | 291 | 33.935 | 35.178 | 66.435 | 1.00 | 28.73 | 6 |
| ATOM | 2317 | CD1 | TYR | A | 291 | 35.025 | 35.596 | 67.191 | 1.00 | 29.72 | 6 |
| ATOM | 2318 | CE1 | TYR | A | 291 | 35.059 | 35.414 | 68.563 | 1.00 | 29.53 | 6 |
| ATOM | 2319 | CD2 | TYR | A | 291 | 32.874 | 34.565 | 67.094 | 1.00 | 27.39 | 6 |
| ATOM | 2320 | CE2 | TYR | A | 291 | 32.898 | 34.377 | 68.466 | 1.00 | 31.03 | 6 |
| ATOM | 2321 | CZ | TYR | A | 291 | 33.997 | 34.808 | 69.194 | 1.00 | 31.85 | 6 |
| ATOM | 2322 | OH | TYR | A | 291 | 34.030 | 34.647 | 70.562 | 1.00 | 38.03 | 8 |
| ATOM | 2323 | C | TYR | A | 291 | 34.527 | 34.345 | 62.745 | 1.00 | 27.99 | 6 |
| ATOM | 2324 | O | TYR | A | 291 | 35.608 | 34.843 | 62.415 | 1.00 | 24.83 | 8 |
| ATOM | 2325 | N | LEU | A | 292 | 33.567 | 34.042 | 61.880 | 1.00 | 30.17 | 7 |
| ATOM | 2326 | CA | LEU | A | 292 | 33.726 | 34.220 | 60.441 | 1.00 | 28.26 | 6 |
| ATOM | 2327 | CB | LEU | A | 292 | 33.561 | 32.861 | 59.741 | 1.00 | 27.70 | 6 |
| ATOM | 2328 | CG | LEU | A | 292 | 34.191 | 31.643 | 60.435 | 1.00 | 24.64 | 6 |
| ATOM | 2329 | CD1 | LEU | A | 292 | 33.867 | 30.380 | 59.661 | 1.00 | 24.66 | 6 |
| ATOM | 2330 | CD2 | LEU | A | 292 | 35.686 | 31.825 | 60.553 | 1.00 | 23.19 | 6 |
| ATOM | 2331 | C | LEU | A | 292 | 32.649 | 35.175 | 59.944 | 1.00 | 25.59 | 6 |
| ATOM | 2332 | O | LEU | A | 292 | 31.640 | 35.394 | 60.611 | 1.00 | 18.11 | 8 |
| ATOM | 2333 | N | GLY | A | 293 | 32.869 | 35.749 | 58.770 | 1.00 | 28.55 | 7 |
| ATOM | 2334 | CA | GLY | A | 293 | 31.878 | 36.653 | 58.223 | 1.00 | 31.26 | 6 |
| ATOM | 2335 | C | GLY | A | 293 | 30.722 | 35.815 | 57.714 | 1.00 | 34.84 | 6 |
| ATOM | 2336 | O | GLY | A | 293 | 30.463 | 34.724 | 58.234 | 1.00 | 34.11 | 8 |
| ATOM | 2337 | N | GLY | A | 294 | 30.036 | 36.312 | 56.689 | 1.00 | 35.34 | 7 |
| ATOM | 2338 | CA | GLY | A | 294 | 28.918 | 35.581 | 56.124 | 1.00 | 34.84 | 6 |
| ATOM | 2339 | C | GLY | A | 294 | 28.142 | 36.445 | 55.155 | 1.00 | 34.79 | 6 |
| ATOM | 2340 | O | GLY | A | 294 | 28.644 | 37.473 | 54.699 | 1.00 | 37.05 | 8 |
| ATOM | 2341 | N | GLY | A | 295 | 26.917 | 36.035 | 54.842 | 1.00 | 31.87 | 7 |
| ATOM | 2342 | CA | GLY | A | 295 | 26.102 | 36.806 | 53.925 | 1.00 | 27.78 | 6 |
| ATOM | 2343 | C | GLY | A | 295 | 25.969 | 38.245 | 54.378 | 1.00 | 27.09 | 6 |
| ATOM | 2344 | O | GLY | A | 295 | 26.192 | 38.558 | 55.546 | 1.00 | 27.03 | 8 |
| ATOM | 2345 | N | GLY | A | 296 | 25.596 | 39.119 | 53.450 | 1.00 | 24.67 | 7 |
| ATOM | 2346 | CA | GLY | A | 296 | 25.440 | 40.527 | 53.757 | 1.00 | 25.28 | 6 |
| ATOM | 2347 | C | GLY | A | 296 | 25.562 | 41.262 | 52.446 | 1.00 | 27.64 | 6 |
| ATOM | 2348 | O | GLY | A | 296 | 26.591 | 41.163 | 51.771 | 1.00 | 26.65 | 8 |
| ATOM | 2349 | N | TYR | A | 297 | 24.526 | 42.009 | 52.078 | 1.00 | 30.21 | 7 |
| ATOM | 2350 | CA | TYR | A | 297 | 24.543 | 42.704 | 50.801 | 1.00 | 30.62 | 6 |
| ATOM | 2351 | CB | TYR | A | 297 | 23.560 | 42.011 | 49.859 | 1.00 | 29.50 | 6 |
| ATOM | 2352 | CG | TYR | A | 297 | 23.717 | 40.516 | 49.953 | 1.00 | 30.33 | 6 |
| ATOM | 2353 | CD1 | TYR | A | 297 | 23.174 | 39.810 | 51.031 | 1.00 | 30.86 | 6 |
| ATOM | 2354 | CE1 | TYR | A | 297 | 23.450 | 38.449 | 51.226 | 1.00 | 30.74 | 6 |
| ATOM | 2355 | CD2 | TYR | A | 297 | 24.538 | 39.824 | 49.062 | 1.00 | 31.20 | 6 |
| ATOM | 2356 | CE2 | TYR | A | 297 | 24.821 | 38.460 | 49.247 | 1.00 | 32.08 | 6 |
| ATOM | 2357 | CZ | TYR | A | 297 | 24.275 | 37.781 | 50.332 | 1.00 | 30.92 | 6 |
| ATOM | 2358 | OH | TYR | A | 297 | 24.539 | 36.440 | 50.509 | 1.00 | 29.60 | 8 |
| ATOM | 2359 | C | TYR | A | 297 | 24.267 | 44.195 | 50.875 | 1.00 | 32.07 | 6 |
| ATOM | 2360 | O | TYR | A | 297 | 24.134 | 44.849 | 49.840 | 1.00 | 33.83 | 8 |
| ATOM | 2361 | N | HIS | A | 298 | 24.180 | 44.725 | 52.094 | 1.00 | 31.41 | 7 |
| ATOM | 2362 | CA | HIS | A | 298 | 23.961 | 46.153 | 52.289 | 1.00 | 33.94 | 6 |
| ATOM | 2363 | CB | HIS | A | 298 | 22.761 | 46.430 | 53.194 | 1.00 | 34.75 | 6 |
| ATOM | 2364 | CG | HIS | A | 298 | 22.379 | 47.880 | 53.256 | 1.00 | 35.16 | 6 |
| ATOM | 2365 | CD2 | HIS | A | 298 | 22.558 | 48.809 | 54.224 | 1.00 | 35.72 | 6 |
| ATOM | 2366 | ND1 | HIS | A | 298 | 21.779 | 48.538 | 52.205 | 1.00 | 34.10 | 7 |
| ATOM | 2367 | CE1 | HIS | A | 298 | 21.605 | 49.809 | 52.522 | 1.00 | 31.84 | 6 |
| ATOM | 2368 | NE2 | HIS | A | 298 | 22.069 | 50.000 | 53.742 | 1.00 | 35.46 | 7 |
| ATOM | 2369 | C | HIS | A | 298 | 25.213 | 46.697 | 52.962 | 1.00 | 36.21 | 6 |
| ATOM | 2370 | O | HIS | A | 298 | 25.471 | 46.405 | 54.133 | 1.00 | 33.83 | 8 |
| ATOM | 2371 | N | PRO | A | 299 | 25.992 | 47.519 | 52.234 | 1.00 | 36.69 | 7 |
| ATOM | 2372 | CD | PRO | A | 299 | 25.680 | 47.997 | 50.881 | 1.00 | 35.57 | 6 |
| ATOM | 2373 | CA | PRO | A | 299 | 27.238 | 48.142 | 52.689 | 1.00 | 35.17 | 6 |
| ATOM | 2374 | CB | PRO | A | 299 | 27.586 | 49.073 | 51.525 | 1.00 | 37.75 | 6 |
| ATOM | 2375 | CG | PRO | A | 299 | 26.216 | 49.399 | 50.954 | 1.00 | 37.76 | 6 |
| ATOM | 2376 | C | PRO | A | 299 | 27.045 | 48.886 | 54.000 | 1.00 | 34.47 | 6 |

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Figure 17-37

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2377 | O | PRO | A | 299 | 27.781 | 48.670 | 54.963 | 1.00 | 33.67 | 8 |
| ATOM | 2378 | N | TYR | A | 300 | 26.051 | 49.763 | 54.026 | 1.00 | 32.69 | 7 |
| ATOM | 2379 | CA | TYR | A | 300 | 25.745 | 50.521 | 55.227 | 1.00 | 32.97 | 6 |
| ATOM | 2380 | CB | TYR | A | 300 | 24.496 | 51.377 | 55.009 | 1.00 | 35.56 | 6 |
| ATOM | 2381 | CG | TYR | A | 300 | 24.648 | 52.524 | 54.028 | 1.00 | 35.96 | 6 |
| ATOM | 2382 | CD1 | TYR | A | 300 | 25.370 | 52.367 | 52.842 | 1.00 | 39.37 | 6 |
| ATOM | 2383 | CE1 | TYR | A | 300 | 25.461 | 53.405 | 51.907 | 1.00 | 39.92 | 6 |
| ATOM | 2384 | CD2 | TYR | A | 300 | 24.016 | 53.752 | 54.259 | 1.00 | 35.92 | 6 |
| ATOM | 2385 | CE2 | TYR | A | 300 | 24.098 | 54.793 | 53.334 | 1.00 | 36.78 | 6 |
| ATOM | 2386 | CZ | TYR | A | 300 | 24.823 | 54.612 | 52.161 | 1.00 | 38.09 | 6 |
| ATOM | 2387 | OH | TYR | A | 300 | 24.927 | 55.634 | 51.251 | 1.00 | 37.68 | 8 |
| ATOM | 2388 | C | TYR | A | 300 | 25.497 | 49.546 | 56.369 | 1.00 | 31.10 | 6 |
| ATOM | 2389 | O | TYR | A | 300 | 26.062 | 49.692 | 57.440 | 1.00 | 30.62 | 8 |
| ATOM | 2390 | N | ALA | A | 301 | 24.661 | 48.541 | 56.125 | 1.00 | 32.55 | 7 |
| ATOM | 2391 | CA | ALA | A | 301 | 24.323 | 47.541 | 57.145 | 1.00 | 31.64 | 6 |
| ATOM | 2392 | CB | ALA | A | 301 | 23.216 | 46.602 | 56.624 | 1.00 | 24.69 | 6 |
| ATOM | 2393 | C | ALA | A | 301 | 25.539 | 46.727 | 57.552 | 1.00 | 30.06 | 6 |
| ATOM | 2394 | O | ALA | A | 301 | 25.848 | 46.579 | 58.734 | 1.00 | 31.91 | 8 |
| ATOM | 2395 | N | LEU | A | 302 | 26.223 | 46.192 | 56.557 | 1.00 | 28.94 | 7 |
| ATOM | 2396 | CA | LEU | A | 302 | 27.404 | 45.383 | 56.795 | 1.00 | 30.55 | 6 |
| ATOM | 2397 | CB | LEU | A | 302 | 28.012 | 45.002 | 55.441 | 1.00 | 31.83 | 6 |
| ATOM | 2398 | CG | LEU | A | 302 | 29.315 | 44.223 | 55.323 | 1.00 | 30.01 | 6 |
| ATOM | 2399 | CD1 | LEU | A | 302 | 29.491 | 43.781 | 53.888 | 1.00 | 32.09 | 6 |
| ATOM | 2400 | CD2 | LEU | A | 302 | 30.475 | 45.077 | 55.762 | 1.00 | 32.23 | 6 |
| ATOM | 2401 | C | LEU | A | 302 | 28.418 | 46.136 | 57.663 | 1.00 | 29.79 | 6 |
| ATOM | 2402 | O | LEU | A | 302 | 28.796 | 45.676 | 58.746 | 1.00 | 27.68 | 8 |
| ATOM | 2403 | N | ALA | A | 303 | 28.842 | 47.299 | 57.179 | 1.00 | 27.92 | 7 |
| ATOM | 2404 | CA | ALA | A | 303 | 29.818 | 48.119 | 57.877 | 1.00 | 25.00 | 6 |
| ATOM | 2405 | CB | ALA | A | 303 | 30.026 | 49.424 | 57.137 | 1.00 | 23.62 | 6 |
| ATOM | 2406 | C | ALA | A | 303 | 29.397 | 48.397 | 59.305 | 1.00 | 25.06 | 6 |
| ATOM | 2407 | O | ALA | A | 303 | 30.088 | 48.015 | 60.248 | 1.00 | 26.90 | 8 |
| ATOM | 2408 | N | ARG | A | 304 | 28.258 | 49.054 | 59.472 | 1.00 | 24.06 | 7 |
| ATOM | 2409 | CA | ARG | A | 304 | 27.794 | 49.382 | 60.810 | 1.00 | 24.37 | 6 |
| ATOM | 2410 | CB | ARG | A | 304 | 26.420 | 50.052 | 60.758 | 1.00 | 23.99 | 6 |
| ATOM | 2411 | CG | ARG | A | 304 | 26.328 | 51.257 | 59.815 | 1.00 | 28.77 | 6 |
| ATOM | 2412 | CD | ARG | A | 304 | 25.106 | 52.089 | 60.156 | 1.00 | 29.96 | 6 |
| ATOM | 2413 | NE | ARG | A | 304 | 23.943 | 51.233 | 60.369 | 1.00 | 36.43 | 7 |
| ATOM | 2414 | CZ | ARG | A | 304 | 22.893 | 51.573 | 61.110 | 1.00 | 37.01 | 6 |
| ATOM | 2415 | NH1 | ARG | A | 304 | 22.854 | 52.757 | 61.713 | 1.00 | 36.37 | 7 |
| ATOM | 2416 | NH2 | ARG | A | 304 | 21.896 | 50.719 | 61.269 | 1.00 | 34.36 | 7 |
| ATOM | 2417 | C | ARG | A | 304 | 27.727 | 48.142 | 61.691 | 1.00 | 24.24 | 6 |
| ATOM | 2418 | O | ARG | A | 304 | 28.343 | 48.099 | 62.762 | 1.00 | 22.34 | 8 |
| ATOM | 2419 | N | ALA | A | 305 | 26.994 | 47.132 | 61.221 | 1.00 | 24.51 | 7 |
| ATOM | 2420 | CA | ALA | A | 305 | 26.801 | 45.883 | 61.959 | 1.00 | 22.70 | 6 |
| ATOM | 2421 | CB | ALA | A | 305 | 25.880 | 44.960 | 61.175 | 1.00 | 18.13 | 6 |
| ATOM | 2422 | C | ALA | A | 305 | 28.089 | 45.142 | 62.351 | 1.00 | 23.33 | 6 |
| ATOM | 2423 | O | ALA | A | 305 | 28.237 | 44.725 | 63.506 | 1.00 | 21.51 | 8 |
| ATOM | 2424 | N | TRP | A | 306 | 29.016 | 44.961 | 61.411 | 1.00 | 22.79 | 7 |
| ATOM | 2425 | CA | TRP | A | 306 | 30.244 | 44.270 | 61.764 | 1.00 | 24.33 | 6 |
| ATOM | 2426 | CB | TRP | A | 306 | 31.029 | 43.842 | 60.524 | 1.00 | 26.93 | 6 |
| ATOM | 2427 | CG | TRP | A | 306 | 30.604 | 42.503 | 59.952 | 1.00 | 27.96 | 6 |
| ATOM | 2428 | CD2 | TRP | A | 306 | 30.861 | 42.013 | 58.629 | 1.00 | 26.38 | 6 |
| ATOM | 2429 | CE2 | TRP | A | 306 | 30.366 | 40.688 | 58.570 | 1.00 | 24.96 | 6 |
| ATOM | 2430 | CE3 | TRP | A | 306 | 31.462 | 42.563 | 57.490 | 1.00 | 23.00 | 6 |
| ATOM | 2431 | CD1 | TRP | A | 306 | 29.983 | 41.484 | 60.620 | 1.00 | 28.53 | 6 |
| ATOM | 2432 | NE1 | TRP | A | 306 | 29.837 | 40.392 | 59.797 | 1.00 | 25.62 | 7 |
| ATOM | 2433 | CZ2 | TRP | A | 306 | 30.450 | 39.904 | 57.414 | 1.00 | 24.51 | 6 |
| ATOM | 2434 | CZ3 | TRP | A | 306 | 31.548 | 41.784 | 56.343 | 1.00 | 25.37 | 6 |
| ATOM | 2435 | CH2 | TRP | A | 306 | 31.042 | 40.465 | 56.315 | 1.00 | 24.20 | 6 |
| ATOM | 2436 | C | TRP | A | 306 | 31.129 | 45.108 | 62.676 | 1.00 | 26.51 | 6 |
| ATOM | 2437 | O | TRP | A | 306 | 31.908 | 44.570 | 63.464 | 1.00 | 25.07 | 8 |
| ATOM | 2438 | N | THR | A | 307 | 31.003 | 46.427 | 62.575 | 1.00 | 28.08 | 7 |
| ATOM | 2439 | CA | THR | A | 307 | 31.785 | 47.323 | 63.415 | 1.00 | 27.91 | 6 |
| ATOM | 2440 | CB | THR | A | 307 | 31.484 | 48.796 | 63.100 | 1.00 | 27.86 | 6 |
| ATOM | 2441 | OG1 | THR | A | 307 | 31.994 | 49.119 | 61.799 | 1.00 | 30.17 | 8 |
| ATOM | 2442 | CG2 | THR | A | 307 | 32.120 | 49.704 | 64.137 | 1.00 | 24.72 | 6 |

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Figure 17-38

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| ATOM | 2443 | C | THR | A | 307 | 31.441 | 47.041 | 64.863 | 1.00 | 29.35 | 6 |
| ATOM | 2444 | O | THR | A | 307 | 32.316 | 46.989 | 65.725 | 1.00 | 32.56 | 8 |
| ATOM | 2445 | N | LEU | A | 308 | 30.159 | 46.857 | 65.135 | 1.00 | 30.60 | 7 |
| ATOM | 2446 | CA | LEU | A | 308 | 29.740 | 46.555 | 66.490 | 1.00 | 33.69 | 6 |
| ATOM | 2447 | CB | LEU | A | 308 | 28.256 | 46.215 | 66.525 | 1.00 | 34.48 | 6 |
| ATOM | 2448 | CG | LEU | A | 308 | 27.338 | 47.337 | 66.058 | 1.00 | 34.79 | 6 |
| ATOM | 2449 | CD1 | LEU | A | 308 | 25.903 | 46.887 | 66.153 | 1.00 | 31.98 | 6 |
| ATOM | 2450 | CD2 | LEU | A | 308 | 27.569 | 48.542 | 66.924 | 1.00 | 36.96 | 6 |
| ATOM | 2451 | C | LEU | A | 308 | 30.531 | 45.353 | 66.965 | 1.00 | 34.57 | 6 |
| ATOM | 2452 | O | LEU | A | 308 | 31.230 | 45.417 | 67.975 | 1.00 | 33.75 | 8 |
| ATOM | 2453 | N | ILE | A | 309 | 30.423 | 44.262 | 66.208 | 1.00 | 35.78 | 7 |
| ATOM | 2454 | CA | ILE | A | 309 | 31.108 | 43.017 | 66.540 | 1.00 | 35.87 | 6 |
| ATOM | 2455 | CB | ILE | A | 309 | 30.939 | 41.949 | 65.431 | 1.00 | 34.95 | 6 |
| ATOM | 2456 | CG2 | ILE | A | 309 | 31.733 | 40.695 | 65.799 | 1.00 | 31.21 | 6 |
| ATOM | 2457 | CG1 | ILE | A | 309 | 29.445 | 41.631 | 65.212 | 1.00 | 34.25 | 6 |
| ATOM | 2458 | CD1 | ILE | A | 309 | 28.726 | 41.014 | 66.407 | 1.00 | 25.04 | 6 |
| ATOM | 2459 | C | ILE | A | 309 | 32.589 | 43.238 | 66.772 | 1.00 | 35.81 | 6 |
| ATOM | 2460 | O | ILE | A | 309 | 33.183 | 42.617 | 67.657 | 1.00 | 38.19 | 8 |
| ATOM | 2461 | N | TRP | A | 310 | 33.197 | 44.111 | 65.977 | 1.00 | 36.10 | 7 |
| ATOM | 2462 | CA | TRP | A | 310 | 34.612 | 44.384 | 66.169 | 1.00 | 35.26 | 6 |
| ATOM | 2463 | CB | TRP | A | 310 | 35.150 | 45.311 | 65.075 | 1.00 | 32.61 | 6 |
| ATOM | 2464 | CG | TRP | A | 310 | 36.619 | 45.588 | 65.220 | 1.00 | 30.79 | 6 |
| ATOM | 2465 | CD2 | TRP | A | 310 | 37.679 | 44.620 | 65.274 | 1.00 | 29.93 | 6 |
| ATOM | 2466 | CE2 | TRP | A | 310 | 38.882 | 45.330 | 65.474 | 1.00 | 28.42 | 6 |
| ATOM | 2467 | CE3 | TRP | A | 310 | 37.731 | 43.224 | 65.174 | 1.00 | 31.59 | 6 |
| ATOM | 2468 | CD1 | TRP | A | 310 | 37.206 | 46.804 | 65.380 | 1.00 | 30.62 | 6 |
| ATOM | 2469 | NE1 | TRP | A | 310 | 38.565 | 46.659 | 65.536 | 1.00 | 29.37 | 7 |
| ATOM | 2470 | CZ2 | TRP | A | 310 | 40.126 | 44.691 | 65.578 | 1.00 | 27.91 | 6 |
| ATOM | 2471 | CZ3 | TRP | A | 310 | 38.978 | 42.585 | 65.279 | 1.00 | 28.06 | 6 |
| ATOM | 2472 | CH2 | TRP | A | 310 | 40.150 | 43.322 | 65.479 | 1.00 | 26.50 | 6 |
| ATOM | 2473 | C | TRP | A | 310 | 34.744 | 45.040 | 67.545 | 1.00 | 36.00 | 6 |
| ATOM | 2474 | O | TRP | A | 310 | 35.365 | 44.476 | 68.440 | 1.00 | 36.24 | 8 |
| ATOM | 2475 | N | CYS | A | 311 | 34.134 | 46.213 | 67.715 | 1.00 | 34.57 | 7 |
| ATOM | 2476 | CA | CYS | A | 311 | 34.183 | 46.937 | 68.985 | 1.00 | 32.82 | 6 |
| ATOM | 2477 | CB | CYS | A | 311 | 33.169 | 48.085 | 68.996 | 1.00 | 35.62 | 6 |
| ATOM | 2478 | SG | CYS | A | 311 | 33.439 | 49.401 | 67.796 | 1.00 | 32.36 | 16 |
| ATOM | 2479 | C | CYS | A | 311 | 33.912 | 46.061 | 70.206 | 1.00 | 32.01 | 6 |
| ATOM | 2480 | O | CYS | A | 311 | 34.452 | 46.313 | 71.280 | 1.00 | 29.82 | 8 |
| ATOM | 2481 | N | GLU | A | 312 | 33.062 | 45.049 | 70.053 | 1.00 | 32.57 | 7 |
| ATOM | 2482 | CA | GLU | A | 312 | 32.731 | 44.159 | 71.171 | 1.00 | 33.86 | 6 |
| ATOM | 2483 | CB | GLU | A | 312 | 31.557 | 43.252 | 70.807 | 1.00 | 34.19 | 6 |
| ATOM | 2484 | CG | GLU | A | 312 | 30.442 | 43.185 | 71.844 | 1.00 | 40.27 | 6 |
| ATOM | 2485 | CD | GLU | A | 312 | 30.923 | 42.821 | 73.239 | 1.00 | 43.80 | 6 |
| ATOM | 2486 | OE1 | GLU | A | 312 | 31.685 | 41.831 | 73.383 | 1.00 | 44.81 | 8 |
| ATOM | 2487 | OE2 | GLU | A | 312 | 30.516 | 43.522 | 74.195 | 1.00 | 41.54 | 8 |
| ATOM | 2488 | C | GLU | A | 312 | 33.953 | 43.298 | 71.456 | 1.00 | 33.77 | 6 |
| ATOM | 2489 | O | GLU | A | 312 | 34.253 | 42.957 | 72.603 | 1.00 | 32.07 | 8 |
| ATOM | 2490 | N | LEU | A | 313 | 34.647 | 42.945 | 70.382 | 1.00 | 33.45 | 7 |
| ATOM | 2491 | CA | LEU | A | 313 | 35.848 | 42.135 | 70.473 | 1.00 | 32.89 | 6 |
| ATOM | 2492 | CB | LEU | A | 313 | 36.172 | 41.513 | 69.115 | 1.00 | 32.14 | 6 |
| ATOM | 2493 | CG | LEU | A | 313 | 35.154 | 40.493 | 68.626 | 1.00 | 27.73 | 6 |
| ATOM | 2494 | CD1 | LEU | A | 313 | 35.587 | 39.956 | 67.269 | 1.00 | 30.39 | 6 |
| ATOM | 2495 | CD2 | LEU | A | 313 | 35.053 | 39.367 | 69.648 | 1.00 | 27.87 | 6 |
| ATOM | 2496 | C | LEU | A | 313 | 36.976 | 43.031 | 70.903 | 1.00 | 31.64 | 6 |
| ATOM | 2497 | O | LEU | A | 313 | 37.605 | 42.793 | 71.925 | 1.00 | 31.74 | 8 |
| ATOM | 2498 | N | SER | A | 314 | 37.206 | 44.064 | 70.099 | 1.00 | 33.49 | 7 |
| ATOM | 2499 | CA | SER | A | 314 | 38.232 | 45.067 | 70.328 | 1.00 | 35.59 | 6 |
| ATOM | 2500 | CB | SER | A | 314 | 38.107 | 46.154 | 69.256 | 1.00 | 36.47 | 6 |
| ATOM | 2501 | OG | SER | A | 314 | 39.141 | 47.120 | 69.353 | 1.00 | 44.55 | 8 |
| ATOM | 2502 | C | SER | A | 314 | 38.046 | 45.661 | 71.730 | 1.00 | 37.82 | 6 |
| ATOM | 2503 | O | SER | A | 314 | 39.015 | 46.043 | 72.395 | 1.00 | 37.32 | 8 |
| ATOM | 2504 | N | GLY | A | 315 | 36.794 | 45.725 | 72.175 | 1.00 | 38.05 | 7 |
| ATOM | 2505 | CA | GLY | A | 315 | 36.506 | 46.243 | 73.498 | 1.00 | 42.42 | 6 |
| ATOM | 2506 | C | GLY | A | 315 | 36.295 | 47.744 | 73.568 | 1.00 | 46.80 | 6 |
| ATOM | 2507 | O | GLY | A | 315 | 35.923 | 48.276 | 74.618 | 1.00 | 47.85 | 8 |
| ATOM | 2508 | N | ARG | A | 316 | 36.518 | 48.438 | 72.458 | 1.00 | 48.90 | 7 |

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| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2509 | CA | ARG | A | 316 | 36.346 | 49.885 | 72.448 | 1.00 | 52.27 | 6 |
| ATOM | 2510 | CB | ARG | A | 316 | 37.144 | 50.479 | 71.283 | 1.00 | 53.60 | 6 |
| ATOM | 2511 | CG | ARG | A | 316 | 36.730 | 50.007 | 69.900 | 1.00 | 52.11 | 6 |
| ATOM | 2512 | CD | ARG | A | 316 | 37.734 | 50.514 | 68.870 | 1.00 | 53.76 | 6 |
| ATOM | 2513 | NE | ARG | A | 316 | 39.028 | 49.854 | 69.019 | 1.00 | 53.67 | 7 |
| ATOM | 2514 | CZ | ARG | A | 316 | 40.135 | 50.221 | 68.383 | 1.00 | 55.34 | 6 |
| ATOM | 2515 | NH1 | ARG | A | 316 | 40.110 | 51.253 | 67.552 | 1.00 | 55.44 | 7 |
| ATOM | 2516 | NH2 | ARG | A | 316 | 41.266 | 49.546 | 68.569 | 1.00 | 55.80 | 7 |
| ATOM | 2517 | C | ARG | A | 316 | 34.882 | 50.343 | 72.391 | 1.00 | 52.06 | 6 |
| ATOM | 2518 | O | ARG | A | 316 | 34.075 | 49.781 | 71.652 | 1.00 | 54.96 | 8 |
| ATOM | 2519 | N | GLU | A | 317 | 34.547 | 51.361 | 73.182 | 1.00 | 51.87 | 7 |
| ATOM | 2520 | CA | GLU | A | 317 | 33.185 | 51.900 | 73.222 | 1.00 | 52.67 | 6 |
| ATOM | 2521 | CB | GLU | A | 317 | 33.111 | 53.139 | 74.123 | 1.00 | 54.70 | 6 |
| ATOM | 2522 | CG | GLU | A | 317 | 32.549 | 52.901 | 75.527 | 1.00 | 60.94 | 6 |
| ATOM | 2523 | CD | GLU | A | 317 | 33.353 | 51.912 | 76.361 | 1.00 | 64.62 | 6 |
| ATOM | 2524 | OE1 | GLU | A | 317 | 33.025 | 51.741 | 77.556 | 1.00 | 64.59 | 8 |
| ATOM | 2525 | OE2 | GLU | A | 317 | 34.305 | 51.302 | 75.832 | 1.00 | 68.64 | 8 |
| ATOM | 2526 | C | GLU | A | 317 | 32.642 | 52.256 | 71.843 | 1.00 | 51.27 | 6 |
| ATOM | 2527 | O | GLU | A | 317 | 33.270 | 52.983 | 71.077 | 1.00 | 49.34 | 8 |
| ATOM | 2528 | N | VAL | A | 318 | 31.457 | 51.733 | 71.548 | 1.00 | 51.30 | 7 |
| ATOM | 2529 | CA | VAL | A | 318 | 30.780 | 51.962 | 70.280 | 1.00 | 48.80 | 6 |
| ATOM | 2530 | CB | VAL | A | 318 | 29.522 | 51.071 | 70.169 | 1.00 | 47.11 | 6 |
| ATOM | 2531 | CG1 | VAL | A | 318 | 28.875 | 51.237 | 68.808 | 1.00 | 45.53 | 6 |
| ATOM | 2532 | CG2 | VAL | A | 318 | 29.895 | 49.631 | 70.424 | 1.00 | 47.05 | 6 |
| ATOM | 2533 | C | VAL | A | 318 | 30.349 | 53.411 | 70.178 | 1.00 | 47.64 | 6 |
| ATOM | 2534 | O | VAL | A | 318 | 29.511 | 53.867 | 70.953 | 1.00 | 47.61 | 8 |
| ATOM | 2535 | N | PRO | A | 319 | 30.925 | 54.165 | 69.234 | 1.00 | 48.14 | 7 |
| ATOM | 2536 | CD | PRO | A | 319 | 31.960 | 53.836 | 68.247 | 1.00 | 48.87 | 6 |
| ATOM | 2537 | CA | PRO | A | 319 | 30.538 | 55.569 | 69.093 | 1.00 | 52.54 | 6 |
| ATOM | 2538 | CB | PRO | A | 319 | 31.438 | 56.051 | 67.954 | 1.00 | 49.96 | 6 |
| ATOM | 2539 | CG | PRO | A | 319 | 31.612 | 54.802 | 67.141 | 1.00 | 50.17 | 6 |
| ATOM | 2540 | C | PRO | A | 319 | 29.052 | 55.679 | 68.764 | 1.00 | 55.84 | 6 |
| ATOM | 2541 | O | PRO | A | 319 | 28.531 | 54.913 | 67.953 | 1.00 | 56.06 | 8 |
| ATOM | 2542 | N | GLU | A | 320 | 28.369 | 56.624 | 69.402 | 1.00 | 59.20 | 7 |
| ATOM | 2543 | CA | GLU | A | 320 | 26.942 | 56.804 | 69.167 | 1.00 | 62.61 | 6 |
| ATOM | 2544 | CB | GLU | A | 320 | 26.302 | 57.588 | 70.313 | 1.00 | 65.59 | 6 |
| ATOM | 2545 | CG | GLU | A | 320 | 26.727 | 59.042 | 70.365 | 1.00 | 73.01 | 6 |
| ATOM | 2546 | CD | GLU | A | 320 | 26.007 | 59.823 | 71.451 | 1.00 | 76.93 | 6 |
| ATOM | 2547 | OE1 | GLU | A | 320 | 24.755 | 59.832 | 71.446 | 1.00 | 77.37 | 8 |
| ATOM | 2548 | OE2 | GLU | A | 320 | 26.697 | 60.431 | 72.303 | 1.00 | 79.46 | 8 |
| ATOM | 2549 | C | GLU | A | 320 | 26.698 | 57.551 | 67.863 | 1.00 | 61.40 | 6 |
| ATOM | 2550 | O | GLU | A | 320 | 25.663 | 58.197 | 67.699 | 1.00 | 62.33 | 8 |
| ATOM | 2551 | N | LYS | A | 321 | 27.650 | 57.463 | 66.939 | 1.00 | 59.47 | 7 |
| ATOM | 2552 | CA | LYS | A | 321 | 27.519 | 58.150 | 65.662 | 1.00 | 59.54 | 6 |
| ATOM | 2553 | CB | LYS | A | 321 | 27.340 | 59.648 | 65.897 | 1.00 | 61.36 | 6 |
| ATOM | 2554 | CG | LYS | A | 321 | 23.620 | 60.323 | 66.366 | 1.00 | 65.23 | 6 |
| ATOM | 2555 | CD | LYS | A | 321 | 19.169 | 59.691 | 67.643 | 1.00 | 66.59 | 6 |
| ATOM | 2556 | CE | LYS | A | 321 | 20.564 | 60.215 | 67.960 | 1.00 | 67.34 | 6 |
| ATOM | 2557 | NZ | LYS | A | 321 | 30.591 | 61.699 | 68.100 | 1.00 | 68.58 | 7 |
| ATOM | 2558 | C | LYS | A | 321 | 28.766 | 57.941 | 64.806 | 1.00 | 59.24 | 6 |
| ATOM | 2559 | O | LYS | A | 321 | 29.845 | 57.623 | 65.319 | 1.00 | 58.70 | 8 |
| ATOM | 2560 | N | LEU | A | 322 | 28.608 | 58.146 | 63.500 | 1.00 | 57.55 | 7 |
| ATOM | 2561 | CA | LEU | A | 322 | 29.702 | 58.002 | 62.543 | 1.00 | 54.72 | 6 |
| ATOM | 2562 | CB | LEU | A | 322 | 29.171 | 57.450 | 61.214 | 1.00 | 52.96 | 6 |
| ATOM | 2563 | CG | LEU | A | 322 | 28.141 | 56.316 | 61.295 | 1.00 | 52.97 | 6 |
| ATOM | 2564 | CD1 | LEU | A | 322 | 27.708 | 55.932 | 59.899 | 1.00 | 49.01 | 6 |
| ATOM | 2565 | CD2 | LEU | A | 322 | 28.716 | 55.115 | 62.035 | 1.00 | 54.73 | 6 |
| ATOM | 2566 | C | LEU | A | 322 | 30.250 | 59.406 | 62.313 | 1.00 | 53.47 | 6 |
| ATOM | 2567 | O | LEU | A | 322 | 29.512 | 60.383 | 62.464 | 1.00 | 53.39 | 8 |
| ATOM | 2568 | N | ASN | A | 323 | 31.530 | 59.521 | 61.965 | 1.00 | 51.43 | 7 |
| ATOM | 2569 | CA | ASN | A | 323 | 32.089 | 60.842 | 61.706 | 1.00 | 50.32 | 6 |
| ATOM | 2570 | CB | ASN | A | 323 | 33.591 | 60.905 | 62.035 | 1.00 | 52.31 | 6 |
| ATOM | 2571 | CG | ASN | A | 323 | 34.428 | 59.964 | 61.189 | 1.00 | 55.06 | 6 |
| ATOM | 2572 | OD1 | ASN | A | 323 | 34.386 | 58.744 | 61.363 | 1.00 | 55.77 | 8 |
| ATOM | 2573 | ND2 | ASN | A | 323 | 35.195 | 60.530 | 60.259 | 1.00 | 52.71 | 7 |
| ATOM | 2574 | C | ASN | A | 323 | 31.843 | 61.199 | 60.243 | 1.00 | 48.63 | 6 |

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Figure 17-40

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 2575 | O | ASN A 323 | 31.135 | 60.479 | 59.538 | 1.00 | 47.52 | 8 |
| ATOM | 2576 | N | ASN A 324 | 32.426 | 62.304 | 59.792 | 1.00 | 47.66 | 7 |
| ATOM | 2577 | CA | ASN A 324 | 32.242 | 62.769 | 58.419 | 1.00 | 49.25 | 6 |
| ATOM | 2578 | CB | ASN A 324 | 32.758 | 64.200 | 58.292 | 1.00 | 50.73 | 6 |
| ATOM | 2579 | CG | ASN A 324 | 32.025 | 65.154 | 59.205 | 1.00 | 53.83 | 6 |
| ATOM | 2580 | OD1 | ASN A 324 | 30.812 | 65.314 | 59.096 | 1.00 | 56.90 | 8 |
| ATOM | 2581 | ND2 | ASN A 324 | 32.755 | 65.789 | 60.119 | 1.00 | 54.93 | 7 |
| ATOM | 2582 | C | ASN A 324 | 32.906 | 61.891 | 57.367 | 1.00 | 49.34 | 6 |
| ATOM | 2583 | O | ASN A 324 | 32.275 | 61.502 | 56.379 | 1.00 | 47.22 | 8 |
| ATOM | 2584 | N | LYS A 325 | 34.182 | 61.590 | 57.586 | 1.00 | 48.27 | 7 |
| ATOM | 2585 | CA | LYS A 325 | 34.957 | 60.759 | 56.676 | 1.00 | 46.57 | 6 |
| ATOM | 2586 | CB | LYS A 325 | 36.314 | 60.453 | 57.305 | 1.00 | 49.94 | 6 |
| ATOM | 2587 | CG | LYS A 325 | 37.299 | 59.737 | 56.399 | 1.00 | 54.75 | 6 |
| ATOM | 2588 | CD | LYS A 325 | 38.562 | 59.329 | 57.173 | 1.00 | 58.22 | 6 |
| ATOM | 2589 | CE | LYS A 325 | 39.236 | 60.521 | 57.844 | 1.00 | 58.35 | 6 |
| ATOM | 2590 | NZ | LYS A 325 | 40.473 | 60.128 | 58.566 | 1.00 | 59.81 | 7 |
| ATOM | 2591 | C | LYS A 325 | 34.202 | 59.458 | 56.410 | 1.00 | 44.85 | 6 |
| ATOM | 2592 | O | LYS A 325 | 34.065 | 59.027 | 55.263 | 1.00 | 43.59 | 8 |
| ATOM | 2593 | N | ALA A 326 | 33.712 | 58.843 | 57.483 | 1.00 | 42.27 | 7 |
| ATOM | 2594 | CA | ALA A 326 | 32.964 | 57.597 | 57.387 | 1.00 | 40.91 | 6 |
| ATOM | 2595 | CB | ALA A 326 | 32.663 | 57.067 | 58.773 | 1.00 | 36.86 | 6 |
| ATOM | 2596 | C | ALA A 326 | 31.666 | 57.803 | 56.612 | 1.00 | 43.30 | 6 |
| ATOM | 2597 | O | ALA A 326 | 31.342 | 57.028 | 55.705 | 1.00 | 42.83 | 8 |
| ATOM | 2598 | N | LYS A 327 | 30.918 | 58.843 | 56.977 | 1.00 | 45.56 | 7 |
| ATOM | 2599 | CA | LYS A 327 | 29.657 | 59.146 | 56.306 | 1.00 | 47.23 | 6 |
| ATOM | 2600 | CB | LYS A 327 | 29.023 | 60.407 | 56.892 | 1.00 | 49.59 | 6 |
| ATOM | 2601 | CG | LYS A 327 | 28.547 | 60.263 | 58.329 | 1.00 | 54.63 | 6 |
| ATOM | 2602 | CD | LYS A 327 | 28.024 | 61.591 | 58.862 | 1.00 | 55.89 | 6 |
| ATOM | 2603 | CE | LYS A 327 | 27.529 | 61.483 | 60.299 | 1.00 | 58.28 | 6 |
| ATOM | 2604 | NZ | LYS A 327 | 26.304 | 60.644 | 60.426 | 1.00 | 59.91 | 7 |
| ATOM | 2605 | C | LYS A 327 | 29.888 | 59.347 | 54.816 | 1.00 | 46.97 | 6 |
| ATOM | 2606 | O | LYS A 327 | 29.090 | 58.913 | 53.990 | 1.00 | 48.10 | 8 |
| ATOM | 2607 | N | GLU A 328 | 30.986 | 60.012 | 54.480 | 1.00 | 44.99 | 7 |
| ATOM | 2608 | CA | GLU A 328 | 31.325 | 60.264 | 53.091 | 1.00 | 43.18 | 6 |
| ATOM | 2609 | CB | GLU A 328 | 32.417 | 61.326 | 53.027 | 1.00 | 47.93 | 6 |
| ATOM | 2610 | CG | GLU A 328 | 31.993 | 62.621 | 53.710 | 1.00 | 53.65 | 6 |
| ATOM | 2611 | CD | GLU A 328 | 33.112 | 63.630 | 53.831 | 1.00 | 55.79 | 6 |
| ATOM | 2612 | OE1 | GLU A 328 | 33.642 | 64.060 | 52.783 | 1.00 | 58.73 | 8 |
| ATOM | 2613 | OE2 | GLU A 328 | 33.459 | 63.991 | 54.979 | 1.00 | 58.13 | 8 |
| ATOM | 2614 | C | GLU A 328 | 31.789 | 58.971 | 52.437 | 1.00 | 41.56 | 6 |
| ATOM | 2615 | O | GLU A 328 | 31.537 | 58.743 | 51.255 | 1.00 | 39.41 | 8 |
| ATOM | 2616 | N | LEU A 329 | 32.465 | 58.123 | 53.211 | 1.00 | 40.64 | 7 |
| ATOM | 2617 | CA | LEU A 329 | 32.940 | 56.844 | 52.695 | 1.00 | 36.45 | 6 |
| ATOM | 2618 | CB | LEU A 329 | 33.623 | 56.032 | 53.801 | 1.00 | 34.70 | 6 |
| ATOM | 2619 | CG | LEU A 329 | 34.100 | 54.610 | 53.433 | 1.00 | 35.69 | 6 |
| ATOM | 2620 | CD1 | LEU A 329 | 35.195 | 54.642 | 52.359 | 1.00 | 30.11 | 6 |
| ATOM | 2621 | CD2 | LEU A 329 | 34.619 | 53.926 | 54.683 | 1.00 | 34.63 | 6 |
| ATOM | 2622 | C | LEU A 329 | 31.746 | 56.064 | 52.157 | 1.00 | 35.77 | 6 |
| ATOM | 2623 | O | LEU A 329 | 31.692 | 55.746 | 50.975 | 1.00 | 34.94 | 8 |
| ATOM | 2624 | N | LEU A 330 | 30.784 | 55.770 | 53.029 | 1.00 | 34.78 | 7 |
| ATOM | 2625 | CA | LEU A 330 | 29.599 | 55.028 | 52.630 | 1.00 | 34.95 | 6 |
| ATOM | 2626 | CB | LEU A 330 | 28.631 | 54.914 | 53.803 | 1.00 | 30.95 | 6 |
| ATOM | 2627 | CG | LEU A 330 | 29.164 | 54.115 | 54.991 | 1.00 | 32.66 | 6 |
| ATOM | 2628 | CD1 | LEU A 330 | 28.051 | 53.904 | 56.022 | 1.00 | 31.74 | 6 |
| ATOM | 2629 | CD2 | LEU A 330 | 29.674 | 52.769 | 54.509 | 1.00 | 30.73 | 6 |
| ATOM | 2630 | C | LEU A 330 | 28.877 | 55.631 | 51.428 | 1.00 | 37.28 | 6 |
| ATOM | 2631 | O | LEU A 330 | 28.395 | 54.901 | 50.557 | 1.00 | 40.56 | 8 |
| ATOM | 2632 | N | LYS A 331 | 28.806 | 56.957 | 51.383 | 1.00 | 38.24 | 7 |
| ATOM | 2633 | CA | LYS A 331 | 28.140 | 57.661 | 50.294 | 1.00 | 39.59 | 6 |
| ATOM | 2634 | CB | LYS A 331 | 27.994 | 59.146 | 50.643 | 1.00 | 42.31 | C |
| ATOM | 2635 | CG | LYS A 331 | 27.129 | 59.399 | 51.873 | 1.00 | 45.93 | 6 |
| ATOM | 2636 | CD | LYS A 331 | 27.017 | 60.879 | 52.244 | 1.00 | 49.72 | 6 |
| ATOM | 2637 | CE | LYS A 331 | 26.271 | 61.698 | 51.193 | 1.00 | 53.66 | 6 |
| ATOM | 2638 | NZ | LYS A 331 | 26.053 | 63.114 | 51.640 | 1.00 | 54.22 | 7 |
| ATOM | 2639 | C | LYS A 331 | 28.863 | 57.514 | 48.958 | 1.00 | 41.02 | 6 |
| ATOM | 2640 | O | LYS A 331 | 28.220 | 57.485 | 47.904 | 1.00 | 39.58 | 8 |

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Figure 17-41

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 2641 | N | SER A 332 | 30.192 | 57.413 | 49.005 | 1.00 | 42.69 | 7 |
| ATOM | 2642 | CA | SER A 332 | 30.998 | 57.274 | 47.792 | 1.00 | 46.02 | 6 |
| ATOM | 2643 | CB | SER A 332 | 32.494 | 57.243 | 48.124 | 1.00 | 47.51 | 6 |
| ATOM | 2644 | OG | SER A 332 | 32.862 | 56.066 | 48.823 | 1.00 | 50.97 | 8 |
| ATOM | 2645 | C | SER A 332 | 30.634 | 56.007 | 47.040 | 1.00 | 48.51 | 6 |
| ATOM | 2646 | O | SER A 332 | 30.706 | 55.959 | 45.811 | 1.00 | 49.45 | 8 |
| ATOM | 2647 | N | ILE A 333 | 30.241 | 54.982 | 47.786 | 1.00 | 51.56 | 7 |
| ATOM | 2648 | CA | ILE A 333 | 29.869 | 53.713 | 47.187 | 1.00 | 54.86 | 6 |
| ATOM | 2649 | CB | ILE A 333 | 29.657 | 52.626 | 48.246 | 1.00 | 55.80 | 6 |
| ATOM | 2650 | CG2 | ILE A 333 | 29.388 | 51.285 | 47.559 | 1.00 | 52.34 | 6 |
| ATOM | 2651 | CG1 | ILE A 333 | 30.892 | 52.522 | 49.140 | 1.00 | 56.89 | 6 |
| ATOM | 2652 | CD1 | ILE A 333 | 30.766 | 51.456 | 50.204 | 1.00 | 60.31 | 6 |
| ATOM | 2653 | C | ILE A 333 | 28.579 | 53.813 | 46.396 | 1.00 | 57.07 | 6 |
| ATOM | 2654 | O | ILE A 333 | 27.572 | 54.321 | 46.897 | 1.00 | 55.59 | 8 |
| ATOM | 2655 | N | ASP A 334 | 28.623 | 53.320 | 45.160 | 1.00 | 61.14 | 7 |
| ATOM | 2656 | CA | ASP A 334 | 27.456 | 53.300 | 44.281 | 1.00 | 65.55 | 6 |
| ATOM | 2657 | CB | ASP A 334 | 27.888 | 53.259 | 42.811 | 1.00 | 69.19 | 6 |
| ATOM | 2658 | CG | ASP A 334 | 28.784 | 52.073 | 42.491 | 1.00 | 70.21 | 6 |
| ATOM | 2659 | OD1 | ASP A 334 | 29.097 | 51.875 | 41.298 | 1.00 | 71.47 | 8 |
| ATOM | 2660 | OD2 | ASP A 334 | 29.181 | 51.344 | 43.427 | 1.00 | 70.91 | 8 |
| ATOM | 2661 | C | ASP A 334 | 26.660 | 52.041 | 44.627 | 1.00 | 65.65 | 6 |
| ATOM | 2662 | O | ASP A 334 | 26.797 | 50.996 | 43.990 | 1.00 | 63.91 | 8 |
| ATOM | 2663 | N | PHE A 335 | 25.822 | 52.153 | 45.649 | 1.00 | 65.73 | 7 |
| ATOM | 2664 | CA | PHE A 335 | 25.041 | 51.021 | 46.104 | 1.00 | 63.44 | 6 |
| ATOM | 2665 | CB | PHE A 335 | 24.980 | 51.034 | 47.632 | 1.00 | 58.05 | 6 |
| ATOM | 2666 | CG | PHE A 335 | 24.039 | 50.028 | 48.195 | 1.00 | 53.82 | 6 |
| ATOM | 2667 | CD1 | PHE A 335 | 24.178 | 48.679 | 47.886 | 1.00 | 52.40 | 6 |
| ATOM | 2668 | CD2 | PHE A 335 | 22.978 | 50.429 | 48.989 | 1.00 | 51.33 | 6 |
| ATOM | 2669 | CE1 | PHE A 335 | 23.265 | 47.742 | 48.356 | 1.00 | 52.73 | 6 |
| ATOM | 2670 | CE2 | PHE A 335 | 22.062 | 49.503 | 49.462 | 1.00 | 53.20 | 6 |
| ATOM | 2671 | CZ | PHE A 335 | 22.204 | 48.151 | 49.144 | 1.00 | 51.76 | 6 |
| ATOM | 2672 | C | PHE A 335 | 23.629 | 50.893 | 45.535 | 1.00 | 65.55 | 6 |
| ATOM | 2673 | O | PHE A 335 | 23.230 | 49.810 | 45.097 | 1.00 | 67.33 | 8 |
| ATOM | 2674 | N | GLU A 336 | 22.874 | 51.986 | 45.537 | 1.00 | 66.47 | 7 |
| ATOM | 2675 | CA | GLU A 336 | 21.497 | 51.948 | 45.048 | 1.00 | 67.43 | 6 |
| ATOM | 2676 | CB | GLU A 336 | 21.422 | 51.379 | 43.626 | 1.00 | 71.79 | 6 |
| ATOM | 2677 | CG | GLU A 336 | 19.982 | 51.245 | 43.116 | 1.00 | 78.77 | 6 |
| ATOM | 2678 | CD | GLU A 336 | 19.868 | 50.505 | 41.789 | 1.00 | 82.67 | 6 |
| ATOM | 2679 | OE1 | GLU A 336 | 20.232 | 49.306 | 41.734 | 1.00 | 83.29 | 8 |
| ATOM | 2680 | OE2 | GLU A 336 | 19.410 | 51.126 | 40.801 | 1.00 | 84.26 | 8 |
| ATOM | 2681 | C | GLU A 336 | 20.655 | 51.069 | 45.971 | 1.00 | 64.72 | 6 |
| ATOM | 2682 | O | GLU A 336 | 20.686 | 49.840 | 45.876 | 1.00 | 59.84 | 8 |
| ATOM | 2683 | N | GLU A 337 | 19.901 | 51.710 | 46.858 | 1.00 | 64.47 | 7 |
| ATOM | 2684 | CA | GLU A 337 | 19.045 | 51.003 | 47.805 | 1.00 | 65.83 | 6 |
| ATOM | 2685 | CB | GLU A 337 | 18.398 | 52.003 | 48.759 | 1.00 | 64.20 | 6 |
| ATOM | 2686 | CG | GLU A 337 | 17.753 | 51.370 | 49.964 | 1.00 | 64.26 | 6 |
| ATOM | 2687 | CD | GLU A 337 | 18.774 | 50.630 | 50.850 | 1.00 | 64.04 | 6 |
| ATOM | 2688 | OE1 | GLU A 337 | 19.741 | 51.322 | 51.261 | 1.00 | 61.66 | 8 |
| ATOM | 2689 | OE2 | GLU A 337 | 18.608 | 49.483 | 51.132 | 1.00 | 63.64 | 8 |
| ATOM | 2690 | C | GLU A 337 | 17.950 | 50.239 | 47.063 | 1.00 | 67.13 | 6 |
| ATOM | 2691 | O | GLU A 337 | 17.269 | 50.807 | 46.205 | 1.00 | 68.27 | 8 |
| ATOM | 2692 | N | PHE A 338 | 17.779 | 48.960 | 47.394 | 1.00 | 67.22 | 7 |
| ATOM | 2693 | CA | PHE A 338 | 16.764 | 48.129 | 46.748 | 1.00 | 68.05 | 6 |
| ATOM | 2694 | CB | PHE A 338 | 16.445 | 46.919 | 47.626 | 1.00 | 69.68 | 6 |
| ATOM | 2695 | CG | PHE A 338 | 15.228 | 46.158 | 47.187 | 1.00 | 72.35 | 6 |
| ATOM | 2696 | CD1 | PHE A 338 | 15.122 | 45.674 | 45.888 | 1.00 | 72.37 | 6 |
| ATOM | 2697 | CD2 | PHE A 338 | 14.172 | 45.941 | 48.074 | 1.00 | 73.61 | 6 |
| ATOM | 2698 | CE1 | PHE A 338 | 13.980 | 44.984 | 45.478 | 1.00 | 73.39 | 6 |
| ATOM | 2699 | CE2 | PHE A 338 | 13.024 | 45.250 | 47.672 | 1.00 | 73.26 | 6 |
| ATOM | 2700 | CZ | PHE A 338 | 12.929 | 44.771 | 46.369 | 1.00 | 73.34 | 6 |
| ATOM | 2701 | C | PHE A 338 | 15.481 | 48.902 | 46.434 | 1.00 | 68.45 | 6 |
| ATOM | 2702 | O | PHE A 338 | 15.286 | 49.367 | 45.310 | 1.00 | 67.92 | 8 |
| ATOM | 2703 | N | ASP A 339 | 14.606 | 49.026 | 47.426 | 1.00 | 68.98 | 7 |
| ATOM | 2704 | CA | ASP A 339 | 13.358 | 49.759 | 47.261 | 1.00 | 70.68 | 6 |
| ATOM | 2705 | CB | ASP A 339 | 12.596 | 49.758 | 48.588 | 1.00 | 71.06 | 6 |
| ATOM | 2706 | CG | ASP A 339 | 11.381 | 50.678 | 48.581 | 1.00 | 72.05 | 6 |

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Figure 17-42

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2707 | OD1 | ASP | A | 339 | 11.548 | 51.893 | 48.320 | 1.00 | 72.29 | 8 |
| ATOM | 2708 | OD2 | ASP | A | 339 | 10.262 | 50.188 | 48.858 | 1.00 | 71.03 | 8 |
| ATOM | 2709 | C | ASP | A | 339 | 13.715 | 51.183 | 46.853 | 1.00 | 73.18 | 6 |
| ATOM | 2710 | O | ASP | A | 339 | 14.407 | 51.884 | 47.592 | 1.00 | 73.78 | 8 |
| ATOM | 2711 | N | ASP | A | 340 | 13.247 | 51.600 | 45.677 | 1.00 | 76.36 | 7 |
| ATOM | 2712 | CA | ASP | A | 340 | 13.518 | 52.943 | 45.152 | 1.00 | 78.34 | 6 |
| ATOM | 2713 | CB | ASP | A | 340 | 12.410 | 53.385 | 44.189 | 1.00 | 77.55 | 6 |
| ATOM | 2714 | CG | ASP | A | 340 | 12.462 | 52.655 | 42.864 | 1.00 | 78.90 | 6 |
| ATOM | 2715 | OD1 | ASP | A | 340 | 12.348 | 51.408 | 42.855 | 1.00 | 78.38 | 8 |
| ATOM | 2716 | OD2 | ASP | A | 340 | 12.620 | 53.336 | 41.830 | 1.00 | 78.74 | 8 |
| ATOM | 2717 | C | ASP | A | 340 | 13.687 | 54.017 | 46.214 | 1.00 | 79.51 | 6 |
| ATOM | 2718 | O | ASP | A | 340 | 14.587 | 54.856 | 46.117 | 1.00 | 80.19 | 8 |
| ATOM | 2719 | N | GLU | A | 341 | 12.824 | 54.000 | 47.224 | 1.00 | 79.64 | 7 |
| ATOM | 2720 | CA | GLU | A | 341 | 12.922 | 54.998 | 48.271 | 1.00 | 80.05 | 6 |
| ATOM | 2721 | CB | GLU | A | 341 | 12.269 | 56.301 | 47.811 | 1.00 | 83.75 | 6 |
| ATOM | 2722 | CG | GLU | A | 341 | 12.411 | 57.442 | 48.806 | 1.00 | 89.02 | 6 |
| ATOM | 2723 | CD | GLU | A | 341 | 11.756 | 58.724 | 48.328 | 1.00 | 91.52 | 6 |
| ATOM | 2724 | OE1 | GLU | A | 341 | 10.515 | 58.738 | 48.175 | 1.00 | 93.33 | 8 |
| ATOM | 2725 | OE2 | GLU | A | 341 | 12.484 | 59.716 | 48.102 | 1.00 | 92.65 | 8 |
| ATOM | 2726 | C | GLU | A | 341 | 12.317 | 54.578 | 49.597 | 1.00 | 77.98 | 6 |
| ATOM | 2727 | O | GLU | A | 341 | 11.102 | 54.610 | 49.777 | 1.00 | 79.82 | 8 |
| ATOM | 2728 | N | VAL | A | 342 | 13.179 | 54.181 | 50.523 | 1.00 | 74.49 | 7 |
| ATOM | 2729 | CA | VAL | A | 342 | 12.745 | 53.793 | 51.859 | 1.00 | 71.55 | 6 |
| ATOM | 2730 | CB | VAL | A | 342 | 13.224 | 52.383 | 52.245 | 1.00 | 72.40 | 6 |
| ATOM | 2731 | CG1 | VAL | A | 342 | 12.672 | 52.004 | 53.610 | 1.00 | 71.16 | 6 |
| ATOM | 2732 | CG2 | VAL | A | 342 | 12.797 | 51.391 | 51.207 | 1.00 | 74.35 | 6 |
| ATOM | 2733 | C | VAL | A | 342 | 13.454 | 54.778 | 52.766 | 1.00 | 68.46 | 6 |
| ATOM | 2734 | O | VAL | A | 342 | 12.952 | 55.154 | 53.829 | 1.00 | 68.96 | 8 |
| ATOM | 2735 | N | ASP | A | 343 | 14.636 | 55.184 | 52.311 | 1.00 | 61.61 | 7 |
| ATOM | 2736 | CA | ASP | A | 343 | 15.486 | 56.114 | 53.029 | 1.00 | 54.91 | 6 |
| ATOM | 2737 | CB | ASP | A | 343 | 14.678 | 57.303 | 53.543 | 1.00 | 55.06 | 6 |
| ATOM | 2738 | CG | ASP | A | 343 | 15.556 | 58.390 | 54.114 | 1.00 | 54.44 | 6 |
| ATOM | 2739 | OD1 | ASP | A | 343 | 15.002 | 59.351 | 54.694 | 1.00 | 56.20 | 8 |
| ATOM | 2740 | OD2 | ASP | A | 343 | 16.795 | 58.287 | 53.969 | 1.00 | 49.32 | 8 |
| ATOM | 2741 | C | ASP | A | 343 | 16.152 | 55.401 | 54.198 | 1.00 | 50.85 | 6 |
| ATOM | 2742 | O | ASP | A | 343 | 15.557 | 55.209 | 55.257 | 1.00 | 49.32 | 8 |
| ATOM | 2743 | N | ARG | A | 344 | 17.396 | 55.004 | 53.980 | 1.00 | 47.84 | 7 |
| ATOM | 2744 | CA | ARG | A | 344 | 18.195 | 54.321 | 54.981 | 1.00 | 45.34 | 6 |
| ATOM | 2745 | CB | ARG | A | 344 | 18.883 | 53.099 | 54.358 | 1.00 | 45.00 | 6 |
| ATOM | 2746 | CG | ARG | A | 344 | 17.950 | 51.969 | 53.974 | 1.00 | 38.03 | 6 |
| ATOM | 2747 | CD | ARG | A | 344 | 17.185 | 51.531 | 55.188 | 1.00 | 35.83 | 6 |
| ATOM | 2748 | NE | ARG | A | 344 | 16.278 | 50.439 | 54.885 | 1.00 | 39.20 | 7 |
| ATOM | 2749 | CZ | ARG | A | 344 | 15.350 | 49.993 | 55.724 | 1.00 | 39.89 | 6 |
| ATOM | 2750 | NH1 | ARG | A | 344 | 15.217 | 50.561 | 56.917 | 1.00 | 40.17 | 7 |
| ATOM | 2751 | NH2 | ARG | A | 344 | 14.566 | 48.976 | 55.375 | 1.00 | 40.75 | 7 |
| ATOM | 2752 | C | ARG | A | 344 | 19.250 | 55.278 | 55.515 | 1.00 | 44.72 | 6 |
| ATOM | 2753 | O | ARG | A | 344 | 20.170 | 54.869 | 56.223 | 1.00 | 46.97 | 8 |
| ATOM | 2754 | N | SER | A | 345 | 19.113 | 56.552 | 55.157 | 1.00 | 45.81 | 7 |
| ATOM | 2755 | CA | SER | A | 345 | 20.045 | 57.596 | 55.577 | 1.00 | 43.66 | 6 |
| ATOM | 2756 | CB | SER | A | 345 | 19.538 | 58.960 | 55.115 | 1.00 | 43.44 | 6 |
| ATOM | 2757 | OG | SER | A | 345 | 18.292 | 59.260 | 55.722 | 1.00 | 45.62 | 8 |
| ATOM | 2758 | C | SER | A | 345 | 20.258 | 57.627 | 57.089 | 1.00 | 42.79 | 6 |
| ATOM | 2759 | O | SER | A | 345 | 21.364 | 57.902 | 57.552 | 1.00 | 42.62 | 8 |
| ATOM | 2760 | N | TYR | A | 346 | 19.200 | 57.354 | 57.851 | 1.00 | 40.55 | 7 |
| ATOM | 2761 | CA | TYR | A | 346 | 19.280 | 57.352 | 59.308 | 1.00 | 41.05 | 6 |
| ATOM | 2762 | CB | TYR | A | 346 | 17.971 | 56.819 | 59.905 | 1.00 | 41.74 | 6 |
| ATOM | 2763 | CG | TYR | A | 346 | 17.668 | 55.355 | 59.630 | 1.00 | 43.47 | 6 |
| ATOM | 2764 | CD1 | TYR | A | 346 | 18.331 | 54.333 | 60.328 | 1.00 | 44.45 | 6 |
| ATOM | 2765 | CE1 | TYR | A | 346 | 18.044 | 52.983 | 60.088 | 1.00 | 41.02 | 6 |
| ATOM | 2766 | CD2 | TYR | A | 346 | 16.710 | 54.988 | 58.682 | 1.00 | 42.08 | 6 |
| ATOM | 2767 | CE2 | TYR | A | 346 | 16.416 | 53.644 | 58.434 | 1.00 | 40.59 | 6 |
| ATOM | 2768 | CZ | TYR | A | 346 | 17.086 | 52.649 | 59.139 | 1.00 | 41.66 | 6 |
| ATOM | 2769 | OH | TYR | A | 346 | 16.806 | 51.324 | 58.884 | 1.00 | 39.60 | 8 |
| ATOM | 2770 | C | TYR | A | 346 | 20.466 | 56.517 | 59.796 | 1.00 | 42.92 | 6 |
| ATOM | 2771 | O | TYR | A | 346 | 21.101 | 56.844 | 60.799 | 1.00 | 42.65 | 8 |
| ATOM | 2772 | N | MET | A | 347 | 20.757 | 55.443 | 59.067 | 1.00 | 44.59 | 7 |

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Figure 17-43

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| ATOM | 2773 | CA | MET | A | 347 | 21.859 | 54.546 | 59.388 | 1.00 | 45.89 | 6 |
| ATOM | 2774 | CB | MET | A | 347 | 21.950 | 53.433 | 58.353 | 1.00 | 45.51 | 6 |
| ATOM | 2775 | CG | MET | A | 347 | 20.727 | 52.567 | 58.244 | 1.00 | 45.01 | 6 |
| ATOM | 2776 | SD | MET | A | 347 | 21.062 | 51.258 | 57.066 | 1.00 | 47.13 | 16 |
| ATOM | 2777 | CE | MET | A | 347 | 21.545 | 52.237 | 55.676 | 1.00 | 44.55 | 6 |
| ATOM | 2778 | C | MET | A | 347 | 23.188 | 55.286 | 59.404 | 1.00 | 48.47 | 6 |
| ATOM | 2779 | O | MET | A | 347 | 24.129 | 54.888 | 60.098 | 1.00 | 49.49 | 8 |
| ATOM | 2780 | N | LEU | A | 348 | 23.259 | 56.351 | 58.610 | 1.00 | 49.03 | 7 |
| ATOM | 2781 | CA | LEU | A | 348 | 24.458 | 57.178 | 58.499 | 1.00 | 48.86 | 6 |
| ATOM | 2782 | CB | LEU | A | 348 | 24.355 | 56.082 | 57.269 | 1.00 | 45.51 | 6 |
| ATOM | 2783 | CG | LEU | A | 348 | 24.280 | 57.424 | 55.895 | 1.00 | 44.47 | 6 |
| ATOM | 2784 | CD1 | LEU | A | 348 | 23.908 | 58.476 | 54.859 | 1.00 | 43.62 | 6 |
| ATOM | 2785 | CD2 | LEU | A | 348 | 25.618 | 56.757 | 55.565 | 1.00 | 42.53 | 6 |
| ATOM | 2786 | C | LEU | A | 348 | 24.644 | 58.049 | 59.738 | 1.00 | 49.33 | 6 |
| ATOM | 2787 | O | LEU | A | 348 | 25.765 | 58.369 | 60.123 | 1.00 | 49.78 | 8 |
| ATOM | 2788 | N | GLU | A | 349 | 23.537 | 58.428 | 60.358 | 1.00 | 48.34 | 7 |
| ATOM | 2789 | CA | GLU | A | 349 | 23.591 | 59.279 | 61.533 | 1.00 | 49.24 | 6 |
| ATOM | 2790 | CB | GLU | A | 349 | 22.198 | 59.848 | 61.811 | 1.00 | 48.36 | 6 |
| ATOM | 2791 | CG | GLU | A | 349 | 21.628 | 60.584 | 60.607 | 1.00 | 45.52 | 6 |
| ATOM | 2792 | CD | GLU | A | 349 | 22.598 | 61.619 | 60.065 | 1.00 | 42.94 | 6 |
| ATOM | 2793 | OE1 | GLU | A | 349 | 22.934 | 62.560 | 60.812 | 1.00 | 40.82 | 8 |
| ATOM | 2794 | OE2 | GLU | A | 349 | 23.028 | 61.483 | 58.900 | 1.00 | 38.30 | 8 |
| ATOM | 2795 | C | GLU | A | 349 | 24.119 | 58.531 | 62.745 | 1.00 | 48.32 | 6 |
| ATOM | 2796 | O | GLU | A | 349 | 25.226 | 58.783 | 63.219 | 1.00 | 47.87 | 8 |
| ATOM | 2797 | N | THR | A | 350 | 23.325 | 57.602 | 63.248 | 1.00 | 48.97 | 7 |
| ATOM | 2798 | CA | THR | A | 350 | 23.744 | 56.832 | 64.398 | 1.00 | 50.70 | 6 |
| ATOM | 2799 | CB | THR | A | 350 | 22.558 | 56.596 | 65.342 | 1.00 | 51.02 | 6 |
| ATOM | 2800 | OG1 | THR | A | 350 | 22.071 | 57.865 | 65.803 | 1.00 | 49.11 | 8 |
| ATOM | 2801 | CG2 | THR | A | 350 | 22.983 | 55.763 | 66.537 | 1.00 | 51.58 | 6 |
| ATOM | 2802 | C | THR | A | 350 | 24.361 | 55.507 | 63.954 | 1.00 | 49.56 | 6 |
| ATOM | 2803 | O | THR | A | 350 | 23.979 | 54.947 | 62.923 | 1.00 | 50.55 | 8 |
| ATOM | 2804 | N | LEU | A | 351 | 25.333 | 55.028 | 64.725 | 1.00 | 46.88 | 7 |
| ATOM | 2805 | CA | LEU | A | 351 | 26.018 | 53.781 | 64.417 | 1.00 | 45.35 | 6 |
| ATOM | 2806 | CB | LEU | A | 351 | 27.342 | 53.726 | 65.185 | 1.00 | 47.05 | 6 |
| ATOM | 2807 | CG | LEU | A | 351 | 28.257 | 52.502 | 65.072 | 1.00 | 49.54 | 6 |
| ATOM | 2808 | CD1 | LEU | A | 351 | 29.575 | 52.777 | 65.766 | 1.00 | 51.50 | 6 |
| ATOM | 2809 | CD2 | LEU | A | 351 | 27.603 | 51.302 | 65.692 | 1.00 | 48.35 | 6 |
| ATOM | 2810 | C | LEU | A | 351 | 25.145 | 52.584 | 64.772 | 1.00 | 44.79 | 6 |
| ATOM | 2811 | O | LEU | A | 351 | 25.131 | 51.578 | 64.061 | 1.00 | 41.45 | 8 |
| ATOM | 2812 | N | LYS | A | 352 | 24.420 | 52.711 | 65.880 | 1.00 | 45.27 | 7 |
| ATOM | 2813 | CA | LYS | A | 352 | 23.531 | 51.662 | 66.375 | 1.00 | 44.62 | 6 |
| ATOM | 2814 | CB | LYS | A | 352 | 23.764 | 51.464 | 67.873 | 1.00 | 42.23 | 6 |
| ATOM | 2815 | CG | LYS | A | 352 | 25.197 | 51.075 | 68.187 | 1.00 | 44.94 | 6 |
| ATOM | 2816 | CD | LYS | A | 352 | 25.572 | 51.262 | 69.650 | 1.00 | 46.80 | 6 |
| ATOM | 2817 | CE | LYS | A | 352 | 24.765 | 50.389 | 70.581 | 1.00 | 45.79 | 6 |
| ATOM | 2818 | NZ | LYS | A | 352 | 25.236 | 50.586 | 71.975 | 1.00 | 47.31 | 7 |
| ATOM | 2819 | C | LYS | A | 352 | 22.096 | 52.087 | 66.116 | 1.00 | 45.12 | 6 |
| ATOM | 2820 | O | LYS | A | 352 | 21.837 | 53.236 | 65.756 | 1.00 | 47.07 | 8 |
| ATOM | 2821 | N | ASP | A | 353 | 21.162 | 51.161 | 66.285 | 1.00 | 44.62 | 7 |
| ATOM | 2822 | CA | ASP | A | 353 | 19.761 | 51.474 | 66.060 | 1.00 | 46.43 | 6 |
| ATOM | 2823 | CB | ASP | A | 353 | 19.302 | 50.943 | 64.692 | 1.00 | 49.38 | 6 |
| ATOM | 2824 | CG | ASP | A | 353 | 19.813 | 49.546 | 64.396 | 1.00 | 51.52 | 6 |
| ATOM | 2825 | OD1 | ASP | A | 353 | 21.028 | 49.396 | 64.158 | 1.00 | 55.36 | 8 |
| ATOM | 2826 | OD2 | ASP | A | 353 | 19.005 | 48.596 | 64.398 | 1.00 | 52.35 | 8 |
| ATOM | 2827 | C | ASP | A | 353 | 18.841 | 50.968 | 67.165 | 1.00 | 45.90 | 6 |
| ATOM | 2828 | O | ASP | A | 353 | 19.152 | 50.001 | 67.854 | 1.00 | 45.98 | 8 |
| ATOM | 2829 | N | PRO | A | 354 | 17.687 | 51.629 | 67.348 | 1.00 | 45.86 | 7 |
| ATOM | 2830 | CD | PRO | A | 354 | 17.162 | 52.775 | 66.587 | 1.00 | 45.36 | 6 |
| ATOM | 2831 | CA | PRO | A | 354 | 16.723 | 51.243 | 68.378 | 1.00 | 45.52 | 6 |
| ATOM | 2832 | CB | PRO | A | 354 | 15.585 | 52.245 | 68.159 | 1.00 | 44.77 | 6 |
| ATOM | 2833 | CG | PRO | A | 354 | 15.681 | 52.513 | 66.664 | 1.00 | 45.06 | 6 |
| ATOM | 2834 | C | PRO | A | 354 | 16.277 | 49.804 | 68.188 | 1.00 | 44.13 | 6 |
| ATOM | 2835 | O | PRO | A | 354 | 16.352 | 49.271 | 67.078 | 1.00 | 42.90 | 8 |
| ATOM | 2836 | N | TRP | A | 355 | 15.821 | 49.174 | 69.267 | 1.00 | 42.77 | 7 |
| ATOM | 2837 | CA | TRP | A | 355 | 15.358 | 47.801 | 69.168 | 1.00 | 43.35 | 6 |
| ATOM | 2838 | CB | TRP | A | 355 | 14.982 | 47.225 | 70.539 | 1.00 | 47.11 | 6 |

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Figure 17-44

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2839 | CG | TRP | A | 355 | 16.168 | 46.752 | 71.322 | 1.00 | 52.43 | 6 |
| ATOM | 2840 | CD2 | TRP | A | 355 | 16.574 | 45.391 | 71.519 | 1.00 | 53.15 | 6 |
| ATOM | 2841 | CE2 | TRP | A | 355 | 17.789 | 45.416 | 72.238 | 1.00 | 54.97 | 6 |
| ATOM | 2842 | CE3 | TRP | A | 355 | 16.031 | 44.153 | 71.155 | 1.00 | 53.39 | 6 |
| ATOM | 2843 | CD1 | TRP | A | 355 | 17.125 | 47.526 | 71.916 | 1.00 | 54.39 | 6 |
| ATOM | 2844 | NE1 | TRP | A | 355 | 18.103 | 46.731 | 72.468 | 1.00 | 57.31 | 7 |
| ATOM | 2845 | CZ2 | TRP | A | 355 | 18.469 | 44.249 | 72.602 | 1.00 | 54.97 | 6 |
| ATOM | 2846 | CZ3 | TRP | A | 355 | 16.706 | 42.995 | 71.518 | 1.00 | 55.77 | 6 |
| ATOM | 2847 | CH2 | TRP | A | 355 | 17.913 | 43.052 | 72.234 | 1.00 | 54.84 | 6 |
| ATOM | 2848 | C | TRP | A | 355 | 14.177 | 47.690 | 68.230 | 1.00 | 41.94 | 6 |
| ATOM | 2849 | O | TRP | A | 355 | 13.508 | 48.677 | 67.915 | 1.00 | 41.39 | 8 |
| ATOM | 2850 | N | ARG | A | 356 | 13.942 | 46.471 | 67.775 | 1.00 | 38.60 | 7 |
| ATOM | 2851 | CA | ARG | A | 356 | 12.855 | 46.185 | 66.866 | 1.00 | 36.55 | 6 |
| ATOM | 2852 | CB | ARG | A | 356 | 13.413 | 46.044 | 65.451 | 1.00 | 35.06 | 6 |
| ATOM | 2853 | CG | ARG | A | 356 | 14.120 | 47.308 | 64.976 | 1.00 | 32.47 | 6 |
| ATOM | 2854 | CD | ARG | A | 356 | 14.969 | 47.082 | 63.733 | 1.00 | 29.54 | 6 |
| ATOM | 2855 | NE | ARG | A | 356 | 15.600 | 48.323 | 63.296 | 1.00 | 28.91 | 7 |
| ATOM | 2856 | CZ | ARG | A | 356 | 16.514 | 48.403 | 62.335 | 1.00 | 30.60 | 6 |
| ATOM | 2857 | NH1 | ARG | A | 356 | 16.916 | 47.305 | 61.702 | 1.00 | 33.52 | 7 |
| ATOM | 2858 | NH2 | ARG | A | 356 | 17.020 | 49.582 | 61.996 | 1.00 | 30.10 | 7 |
| ATOM | 2859 | C | ARG | A | 356 | 12.270 | 44.879 | 67.361 | 1.00 | 36.01 | 6 |
| ATOM | 2860 | O | ARG | A | 356 | 12.447 | 43.831 | 66.742 | 1.00 | 38.38 | 8 |
| ATOM | 2861 | N | GLY | A | 357 | 11.587 | 44.949 | 68.499 | 1.00 | 36.04 | 7 |
| ATOM | 2862 | CA | GLY | A | 357 | 11.001 | 43.758 | 69.085 | 1.00 | 36.08 | 6 |
| ATOM | 2863 | C | GLY | A | 357 | 9.514 | 43.596 | 68.851 | 1.00 | 34.51 | 6 |
| ATOM | 2864 | O | GLY | A | 357 | 8.943 | 44.196 | 67.943 | 1.00 | 36.77 | 8 |
| ATOM | 2865 | N | GLY | A | 358 | 8.892 | 42.772 | 69.687 | 1.00 | 36.04 | 7 |
| ATOM | 2866 | CA | GLY | A | 358 | 7.466 | 42.506 | 69.593 | 1.00 | 32.26 | 6 |
| ATOM | 2867 | C | GLY | A | 358 | 7.106 | 41.263 | 70.385 | 1.00 | 29.85 | 6 |
| ATOM | 2868 | O | GLY | A | 358 | 7.832 | 40.839 | 71.288 | 1.00 | 28.86 | 8 |
| ATOM | 2869 | N | GLU | A | 359 | 5.975 | 40.667 | 70.055 | 1.00 | 30.88 | 7 |
| ATOM | 2870 | CA | GLU | A | 359 | 5.550 | 39.455 | 70.743 | 1.00 | 32.58 | 6 |
| ATOM | 2871 | CB | GLU | A | 359 | 4.034 | 39.289 | 70.604 | 1.00 | 38.60 | 6 |
| ATOM | 2872 | CG | GLU | A | 359 | 3.230 | 40.435 | 71.222 | 1.00 | 47.44 | 6 |
| ATOM | 2873 | CD | GLU | A | 359 | 1.957 | 40.762 | 70.445 | 1.00 | 50.93 | 6 |
| ATOM | 2874 | OE1 | GLU | A | 359 | 1.123 | 39.852 | 70.221 | 1.00 | 52.13 | 8 |
| ATOM | 2875 | OE2 | GLU | A | 359 | 1.798 | 41.942 | 70.061 | 1.00 | 51.03 | 8 |
| ATOM | 2876 | C | GLU | A | 359 | 6.250 | 38.275 | 70.091 | 1.00 | 28.29 | 6 |
| ATOM | 2877 | O | GLU | A | 359 | 6.790 | 38.382 | 68.997 | 1.00 | 27.88 | 8 |
| ATOM | 2878 | N | VAL | A | 360 | 6.263 | 37.147 | 70.772 | 1.00 | 27.97 | 7 |
| ATOM | 2879 | CA | VAL | A | 360 | 6.859 | 35.957 | 70.193 | 1.00 | 25.86 | 6 |
| ATOM | 2880 | CB | VAL | A | 360 | 7.673 | 35.168 | 71.237 | 1.00 | 22.02 | 6 |
| ATOM | 2881 | CG1 | VAL | A | 360 | 8.155 | 33.849 | 70.641 | 1.00 | 19.45 | 6 |
| ATOM | 2882 | CG2 | VAL | A | 360 | 8.850 | 36.009 | 71.698 | 1.00 | 17.88 | 6 |
| ATOM | 2883 | C | VAL | A | 360 | 5.703 | 35.099 | 69.670 | 1.00 | 28.04 | 6 |
| ATOM | 2884 | C | VAL | A | 360 | 4.842 | 34.655 | 70.440 | 1.00 | 27.34 | 8 |
| ATOM | 2885 | N | ARG | A | 361 | 5.663 | 34.898 | 68.358 | 1.00 | 27.70 | 7 |
| ATOM | 2886 | C. | ARG | A | 361 | 4.612 | 34.091 | 67.765 | 1.00 | 32.85 | 6 |
| ATOM | 2887 | CB | ARG | A | 361 | 4.693 | 34.164 | 66.242 | 1.00 | 32.30 | 6 |
| ATOM | 2888 | CG | ARG | A | 361 | 4.243 | 35.504 | 65.687 | 1.00 | 38.81 | 6 |
| ATOM | 2889 | CD | ARG | A | 361 | 4.546 | 35.653 | 64.201 | 1.00 | 40.09 | 6 |
| ATOM | 2890 | NE | ARG | A | 361 | 5.974 | 35.812 | 63.961 | 1.00 | 38.77 | 7 |
| ATOM | 2891 | CZ | ARG | A | 361 | 6.514 | 35.989 | 62.763 | 1.00 | 39.21 | 6 |
| ATOM | 2892 | NH1 | ARG | A | 361 | 5.748 | 36.027 | 61.685 | 1.00 | 40.79 | 7 |
| ATOM | 2893 | NH2 | ARG | A | 361 | 7.822 | 36.145 | 62.643 | 1.00 | 42.94 | 7 |
| ATOM | 2894 | C | ARG | A | 361 | 4.689 | 32.638 | 68.222 | 1.00 | 35.65 | 6 |
| ATOM | 2895 | O | ARG | A | 361 | 5.768 | 32.097 | 68.471 | 1.00 | 37.08 | 8 |
| ATOM | 2896 | N | LYS | A | 362 | 3.526 | 32.017 | 68.347 | 1.00 | 37.80 | 7 |
| ATOM | 2897 | CA | LYS | A | 362 | 3.436 | 30.626 | 68.757 | 1.00 | 39.91 | 6 |
| ATOM | 2898 | CB | LYS | A | 362 | 1.982 | 30.152 | 68.648 | 1.00 | 43.43 | 6 |
| ATOM | 2899 | CG | LYS | A | 362 | 1.014 | 30.803 | 69.640 | 1.00 | 45.11 | 6 |
| ATOM | 2900 | CD | LYS | A | 362 | 1.117 | 32.346 | 69.673 | 1.00 | 49.43 | 6 |
| ATOM | 2901 | CE | LYS | A | 362 | 0.813 | 33.022 | 68.327 | 1.00 | 45.02 | 6 |
| ATOM | 2902 | NZ | LYS | A | 362 | 0.962 | 34.509 | 68.422 | 1.00 | 41.08 | 7 |
| ATOM | 2903 | C | LYS | A | 362 | 4.320 | 29.809 | 67.831 | 1.00 | 39.25 | 6 |
| ATOM | 2904 | O | LYS | A | 362 | 4.953 | 28.835 | 68.248 | 1.00 | 35.45 | 8 |

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Figure 17-45

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 2905 | N | GLU A 363 | 4.358 | 30.229 | 66.568 | 1.00 | 41.13 | 7 |
| ATOM | 2906 | CA | GLU A 363 | 5.147 | 29.554 | 65.539 | 1.00 | 43.96 | 6 |
| ATOM | 2907 | CB | GLU A 363 | 5.225 | 30.416 | 64.278 | 1.00 | 45.90 | 6 |
| ATOM | 2908 | CG | GLU A 363 | 3.892 | 30.876 | 63.741 | 1.00 | 50.68 | 6 |
| ATOM | 2909 | CD | GLU A 363 | 4.045 | 31.738 | 62.507 | 1.00 | 54.11 | 6 |
| ATOM | 2910 | OE1 | GLU A 363 | 4.571 | 31.224 | 61.494 | 1.00 | 53.90 | 8 |
| ATOM | 2911 | OE2 | GLU A 363 | 3.648 | 32.927 | 62.552 | 1.00 | 56.05 | 8 |
| ATOM | 2912 | C | GLU A 363 | 6.558 | 29.296 | 66.046 | 1.00 | 42.39 | 6 |
| ATOM | 2913 | O | GLU A 363 | 7.062 | 28.169 | 65.989 | 1.00 | 41.48 | 8 |
| ATOM | 2914 | N | VAL A 364 | 7.183 | 30.360 | 66.540 | 1.00 | 37.27 | 7 |
| ATOM | 2915 | CA | VAL A 364 | 8.535 | 30.291 | 67.064 | 1.00 | 35.30 | 6 |
| ATOM | 2916 | CB | VAL A 364 | 9.038 | 31.696 | 67.469 | 1.00 | 36.88 | 6 |
| ATOM | 2917 | CG1 | VAL A 364 | 10.444 | 31.599 | 68.043 | 1.00 | 37.77 | 6 |
| ATOM | 2918 | CG2 | VAL A 364 | 9.018 | 32.628 | 66.252 | 1.00 | 34.78 | 6 |
| ATOM | 2919 | C | VAL A 364 | 8.650 | 29.361 | 68.268 | 1.00 | 33.01 | 6 |
| ATOM | 2920 | O | VAL A 364 | 9.622 | 28.614 | 68.379 | 1.00 | 31.55 | 8 |
| ATOM | 2921 | N | LYS A 365 | 7.664 | 29.409 | 69.165 | 1.00 | 32.61 | 7 |
| ATOM | 2922 | CA | LYS A 365 | 7.674 | 28.567 | 70.362 | 1.00 | 30.96 | 6 |
| ATOM | 2923 | CB | LYS A 365 | 6.598 | 29.010 | 71.358 | 1.00 | 30.13 | 6 |
| ATOM | 2924 | CG | LYS A 365 | 6.826 | 30.409 | 71.899 | 1.00 | 36.02 | 6 |
| ATOM | 2925 | CD | LYS A 365 | 5.837 | 30.781 | 72.995 | 1.00 | 38.94 | 6 |
| ATOM | 2926 | CE | LYS A 365 | 6.120 | 32.187 | 73.509 | 1.00 | 41.58 | 6 |
| ATOM | 2927 | NZ | LYS A 365 | 5.191 | 32.611 | 74.585 | 1.00 | 44.29 | 7 |
| ATOM | 2928 | C | LYS A 365 | 7.452 | 27.114 | 70.007 | 1.00 | 30.32 | 6 |
| ATOM | 2929 | O | LYS A 365 | 8.195 | 26.237 | 70.442 | 1.00 | 31.32 | 8 |
| ATOM | 2930 | N | ASP A 366 | 6.427 | 26.863 | 69.209 | 1.00 | 29.85 | 7 |
| ATOM | 2931 | CA | ASP A 366 | 6.115 | 25.509 | 68.807 | 1.00 | 32.07 | 6 |
| ATOM | 2932 | CB | ASP A 366 | 4.948 | 25.522 | 67.818 | 1.00 | 35.98 | 6 |
| ATOM | 2933 | CG | ASP A 366 | 3.711 | 26.206 | 68.381 | 1.00 | 39.88 | 6 |
| ATOM | 2934 | OD1 | ASP A 366 | 3.124 | 25.692 | 69.359 | 1.00 | 40.16 | 8 |
| ATOM | 2935 | OD2 | ASP A 366 | 3.326 | 27.266 | 67.848 | 1.00 | 43.21 | 8 |
| ATOM | 2936 | C | ASP A 366 | 7.343 | 24.866 | 68.161 | 1.00 | 33.07 | 6 |
| ATOM | 2937 | O | ASP A 366 | 7.753 | 23.763 | 68.540 | 1.00 | 32.64 | 8 |
| ATOM | 2938 | N | THR A 367 | 7.932 | 25.565 | 67.193 | 1.00 | 31.89 | 7 |
| ATOM | 2939 | CA | THR A 367 | 9.088 | 25.045 | 66.490 | 1.00 | 31.17 | 6 |
| ATOM | 2940 | CB | THR A 367 | 9.712 | 26.070 | 65.572 | 1.00 | 31.55 | 6 |
| ATOM | 2941 | OG1 | THR A 367 | 8.707 | 26.620 | 64.714 | 1.00 | 34.37 | 8 |
| ATOM | 2942 | CG2 | THR A 367 | 10.780 | 25.404 | 64.723 | 1.00 | 33.55 | 6 |
| ATOM | 2943 | C | THR A 367 | 10.146 | 24.633 | 67.472 | 1.00 | 33.09 | 6 |
| ATOM | 2944 | O | THR A 367 | 10.586 | 23.476 | 67.485 | 1.00 | 38.62 | 8 |
| ATOM | 2945 | N | LEU A 368 | 10.570 | 25.579 | 68.298 | 1.00 | 31.85 | 7 |
| ATOM | 2946 | CA | LEU A 368 | 11.582 | 25.264 | 69.288 | 1.00 | 32.87 | 6 |
| ATOM | 2947 | CB | LEU A 368 | 11.848 | 26.478 | 70.179 | 1.00 | 27.73 | 6 |
| ATOM | 2948 | CG | LEU A 368 | 12.887 | 27.449 | 69.588 | 1.00 | 29.05 | 6 |
| ATOM | 2949 | CD1 | LEU A 368 | 14.260 | 26.777 | 69.541 | 1.00 | 23.05 | 6 |
| ATOM | 2950 | CD2 | LEU A 368 | 12.473 | 27.896 | 68.193 | 1.00 | 26.53 | 6 |
| ATOM | 2951 | C | LEU A 368 | 11.157 | 24.053 | 70.107 | 1.00 | 35.16 | 6 |
| ATOM | 2952 | O | LEU A 368 | 11.910 | 23.077 | 70.217 | 1.00 | 35.18 | 8 |
| ATOM | 2953 | N | GLU A 369 | 9.942 | 24.101 | 70.649 | 1.00 | 37.56 | 7 |
| ATOM | 2954 | CA | GLU A 369 | 9.431 | 22.993 | 71.442 | 1.00 | 40.23 | 6 |
| ATOM | 2955 | CB | GLU A 369 | 7.956 | 23.216 | 71.770 | 1.00 | 42.07 | 6 |
| ATOM | 2956 | CG | GLU A 369 | 7.722 | 24.460 | 72.617 | 1.00 | 48.51 | 6 |
| ATOM | 2957 | CD | GLU A 369 | 6.281 | 24.616 | 73.067 | 1.00 | 51.93 | 6 |
| ATOM | 2958 | OE1 | GLU A 369 | 5.777 | 23.724 | 73.782 | 1.00 | 52.84 | 8 |
| ATOM | 2959 | OE2 | GLU A 369 | 5.652 | 25.636 | 72.710 | 1.00 | 58.33 | 8 |
| ATOM | 2960 | C | GLU A 369 | 9.633 | 21.672 | 70.701 | 1.00 | 41.14 | 6 |
| ATOM | 2961 | O | GLU A 369 | 10.087 | 20.684 | 71.286 | 1.00 | 41.87 | 8 |
| ATOM | 2962 | N | LYS A 370 | 9.309 | 21.653 | 69.411 | 1.00 | 39.65 | 7 |
| ATOM | 2963 | CA | LYS A 370 | 9.497 | 20.443 | 68.636 | 1.00 | 38.26 | 6 |
| ATOM | 2964 | CB | LYS A 370 | 9.144 | 20.654 | 67.166 | 1.00 | 40.63 | 6 |
| ATOM | 2965 | CG | LYS A 370 | 7.675 | 20.597 | 66.854 | 1.00 | 44.49 | 6 |
| ATOM | 2966 | CD | LYS A 370 | 7.495 | 20.358 | 65.363 | 1.00 | 49.95 | 6 |
| ATOM | 2967 | CE | LYS A 370 | 6.052 | 20.023 | 65.015 | 1.00 | 54.28 | 6 |
| ATOM | 2968 | NZ | LYS A 370 | 5.890 | 19.679 | 63.574 | 1.00 | 55.44 | 7 |
| ATOM | 2969 | C | LYS A 370 | 10.948 | 20.034 | 68.730 | 1.00 | 37.85 | 6 |
| ATOM | 2970 | O | LYS A 370 | 11.261 | 18.930 | 69.156 | 1.00 | 37.95 | 8 |

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Figure 17-46

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2971 | N | ALA | A | 371 | 11.827 | 20.944 | 68.325 | 1.00 | 37.78 | 7 |
| ATOM | 2972 | CA | ALA | A | 371 | 13.264 | 20.704 | 68.340 | 1.00 | 36.39 | 6 |
| ATOM | 2973 | CB | ALA | A | 371 | 14.007 | 22.030 | 68.200 | 1.00 | 37.73 | 6 |
| ATOM | 2974 | C | ALA | A | 371 | 13.719 | 19.972 | 69.603 | 1.00 | 35.42 | 6 |
| ATOM | 2975 | O | ALA | A | 371 | 14.424 | 18.964 | 69.525 | 1.00 | 32.06 | 8 |
| ATOM | 2976 | N | ALA | A | 372 | 13.317 | 20.478 | 70.766 | 1.00 | 33.96 | 7 |
| ATOM | 2977 | CA | ALA | A | 372 | 13.695 | 19.848 | 72.024 | 1.00 | 32.22 | 6 |
| ATOM | 2978 | CB | ALA | A | 372 | 12.946 | 20.486 | 73.165 | 1.00 | 28.27 | 6 |
| ATOM | 2979 | C | ALA | A | 372 | 13.372 | 18.362 | 71.953 | 1.00 | 31.75 | 6 |
| ATOM | 2980 | O | ALA | A | 372 | 14.183 | 17.517 | 72.338 | 1.00 | 31.56 | 8 |
| ATOM | 2981 | N | ALA | A | 373 | 12.187 | 18.059 | 71.432 | 1.00 | 32.72 | 7 |
| ATOM | 2982 | CA | ALA | A | 373 | 11.710 | 16.684 | 71.305 | 1.00 | 32.32 | 6 |
| ATOM | 2983 | CB | ALA | A | 373 | 10.206 | 16.689 | 71.103 | 1.00 | 30.18 | 6 |
| ATOM | 2984 | C | ALA | A | 373 | 12.385 | 15.921 | 70.172 | 1.00 | 33.13 | 6 |
| ATOM | 2985 | OT1 | ALA | A | 373 | 13.078 | 14.926 | 70.468 | 1.00 | 35.87 | 8 |
| ATOM | 2986 | OT2 | ALA | A | 373 | 12.218 | 16.320 | 69.003 | 1.00 | 34.11 | 8 |
| ATOM | 2987 | ZN | ZN | Z | 951 | 22.693 | 34.497 | 53.990 | 1.00 | 36.45 | 6 |
| ATOM | 2988 | OH2 | WAT | S | 1 | 35.654 | 44.211 | 49.416 | 1.00 | 9.27 | 8 |
| ATOM | 2989 | OH2 | WAT | S | 2 | 24.480 | 33.130 | 53.069 | 1.00 | 21.27 | 8 |
| ATOM | 2990 | OH2 | WAT | S | 3 | 22.124 | 30.277 | 59.314 | 1.00 | 14.69 | 8 |
| ATOM | 2991 | OH2 | WAT | S | 4 | 13.839 | 20.611 | 75.741 | 1.00 | 27.94 | 8 |
| ATOM | 2992 | OH2 | WAT | S | 5 | 34.033 | 41.903 | 46.522 | 1.00 | 44.54 | 8 |
| ATOM | 2993 | OH2 | WAT | S | 6 | 15.039 | 42.130 | 55.781 | 1.00 | 23.79 | 8 |
| ATOM | 2994 | OH2 | WAT | S | 7 | 32.737 | 41.397 | 75.900 | 1.00 | 15.80 | 8 |
| ATOM | 2995 | OH2 | WAT | S | 8 | 11.367 | 22.606 | 58.814 | 1.00 | 23.37 | 8 |
| ATOM | 2996 | OH2 | WAT | S | 9 | 13.909 | 18.160 | 65.105 | 1.00 | 29.93 | 8 |
| ATOM | 2997 | OH2 | WAT | S | 10 | 29.655 | 56.108 | 58.029 | 1.00 | 50.54 | 8 |
| ATOM | 2998 | OH2 | WAT | S | 11 | 45.405 | 17.964 | 51.885 | 1.00 | 9.28 | 8 |
| ATOM | 2999 | OH2 | WAT | S | 12 | 21.870 | 35.873 | 34.515 | 1.00 | 32.78 | 8 |
| ATOM | 3000 | OH2 | WAT | S | 13 | 43.504 | 35.670 | 33.779 | 1.00 | 28.85 | 8 |
| ATOM | 3001 | OH2 | WAT | S | 14 | 2.054 | 37.997 | 68.430 | 1.00 | 40.53 | 8 |
| ATOM | 3002 | OH2 | WAT | S | 15 | 49.730 | 28.024 | 55.966 | 1.00 | 21.42 | 8 |
| ATOM | 3003 | OH2 | WAT | S | 16 | 47.503 | 32.289 | 34.336 | 1.00 | 26.13 | 8 |
| ATOM | 3004 | OH2 | WAT | S | 17 | 6.101 | 26.102 | 64.434 | 1.00 | 21.69 | 8 |
| ATOM | 3005 | OH2 | WAT | S | 18 | 10.761 | 46.748 | 45.836 | 1.00 | 15.79 | 8 |
| ATOM | 3006 | OH2 | WAT | S | 19 | 9.146 | 16.861 | 61.441 | 1.00 | 16.68 | 8 |
| ATOM | 3007 | OH2 | WAT | S | 20 | 5.684 | 34.080 | 76.599 | 1.00 | 37.53 | 8 |
| ATOM | 3008 | OH2 | WAT | S | 21 | 14.896 | 33.163 | 49.117 | 1.00 | 34.17 | 8 |
| ATOM | 3009 | OH2 | WAT | S | 22 | 43.346 | 40.839 | 36.825 | 1.00 | 35.64 | 8 |
| ATOM | 3010 | OH2 | WAT | S | 23 | 0.516 | 27.705 | 69.174 | 1.00 | 21.02 | 8 |
| ATOM | 3011 | OH2 | WAT | S | 24 | 41.270 | 25.444 | 29.717 | 1.00 | 29.80 | 8 |
| ATOM | 3012 | OH2 | WAT | S | 25 | 17.818 | 29.142 | 54.584 | 1.00 | 27.92 | 8 |
| ATOM | 3013 | OH2 | WAT | S | 26 | 21.512 | 60.572 | 56.912 | 1.00 | 16.77 | 8 |
| ATOM | 3014 | OH2 | WAT | S | 27 | 21.211 | 33.582 | 48.347 | 1.00 | 23.93 | 8 |
| ATOM | 3015 | OH2 | WAT | S | 28 | 47.805 | 24.638 | 56.619 | 1.00 | 23.73 | 8 |
| ATOM | 3016 | OH2 | WAT | S | 29 | 44.624 | 50.302 | 58.154 | 1.00 | 16.79 | 8 |
| ATOM | 3017 | OH2 | WAT | S | 30 | 31.096 | 16.437 | 51.311 | 1.00 | 26.61 | 8 |
| ATOM | 3018 | OH2 | WAT | S | 31 | 39.837 | 38.833 | 55.145 | 1.00 | 32.28 | 8 |
| ATOM | 3019 | OH2 | WAT | S | 32 | 11.660 | 43.601 | 63.704 | 1.00 | 22.94 | 8 |
| ATOM | 3020 | OH2 | WAT | S | 33 | 49.899 | 23.474 | 53.058 | 1.00 | 26.85 | 8 |
| ATOM | 3021 | OH2 | WAT | S | 34 | 34.624 | 17.734 | 32.228 | 1.00 | 21.18 | 8 |
| ATOM | 3022 | OH2 | WAT | S | 35 | 26.926 | 15.913 | 62.444 | 1.00 | 27.01 | 8 |
| ATOM | 3023 | OH2 | WAT | S | 36 | 8.893 | 28.686 | 63.905 | 1.00 | 27.68 | 8 |
| ATOM | 3024 | OH2 | WAT | S | 37 | 23.381 | 26.634 | 43.532 | 1.00 | 24.42 | 8 |
| ATOM | 3025 | OH2 | WAT | S | 38 | 48.484 | 27.990 | 65.270 | 1.00 | 34.86 | 8 |
| ATOM | 3026 | OH2 | WAT | S | 39 | 43.382 | 28.410 | 74.379 | 1.00 | 25.68 | 8 |
| ATOM | 3027 | OH2 | WAT | S | 40 | 42.904 | 18.967 | 70.272 | 1.00 | 29.45 | 8 |
| ATOM | 3028 | OH2 | WAT | S | 41 | 20.521 | 53.828 | 50.298 | 1.00 | 22.35 | 8 |
| ATOM | 3029 | OH2 | WAT | S | 42 | 13.310 | 38.921 | 48.404 | 1.00 | 23.32 | 8 |
| ATOM | 3030 | OH2 | WAT | S | 43 | 9.787 | 46.265 | 60.012 | 1.00 | 33.51 | 8 |
| ATOM | 3031 | OH2 | WAT | S | 44 | 36.089 | 30.416 | 51.377 | 1.00 | 47.75 | 8 |
| ATOM | 3032 | OH2 | WAT | S | 45 | 14.831 | 48.131 | 42.151 | 1.00 | 50.96 | 8 |
| ATOM | 3033 | OH2 | WAT | S | 46 | 54.162 | 48.194 | 60.971 | 1.00 | 22.66 | 8 |
| ATOM | 3034 | OH2 | WAT | S | 47 | 38.943 | 61.290 | 63.509 | 1.00 | 33.73 | 8 |
| ATOM | 3035 | OH2 | WAT | S | 48 | 29.980 | 18.112 | 33.130 | 1.00 | 35.80 | 8 |
| ATOM | 3036 | OH2 | WAT | S | 49 | 31.879 | 50.673 | 44.528 | 1.00 | 24.39 | 8 |

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Figure 17-47

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3037 | OH2 | WAT | S | 50 | 39.863 | 14.629 | 64.307 | 1.00 | 24.19 | 8 |
| ATOM | 3038 | OH2 | WAT | S | 51 | 26.119 | 29.471 | 38.549 | 1.00 | 27.78 | 8 |
| ATOM | 3039 | OH2 | WAT | S | 52 | 48.070 | 41.589 | 44.011 | 1.00 | 36.38 | 8 |
| ATOM | 3040 | OH2 | WAT | S | 53 | 50.802 | 29.649 | 52.495 | 1.00 | 31.04 | 8 |
| ATOM | 3041 | OH2 | WAT | S | 54 | 49.540 | 35.532 | 71.585 | 1.00 | 20.96 | 8 |
| ATOM | 3042 | OH2 | WAT | S | 55 | 6.887 | 23.426 | 64.961 | 1.00 | 17.49 | 8 |
| ATOM | 3043 | OH2 | WAT | S | 56 | 25.698 | 39.891 | 37.674 | 1.00 | 51.51 | 8 |
| ATOM | 3044 | OH2 | WAT | S | 57 | 45.498 | 44.101 | 55.393 | 1.00 | 37.34 | 8 |
| ATOM | 3045 | OH2 | WAT | S | 58 | 44.661 | 34.733 | 46.902 | 1.00 | 44.52 | 8 |
| ATOM | 3046 | OH2 | WAT | S | 59 | 21.912 | 21.320 | 79.233 | 1.00 | 26.96 | 8 |
| ATOM | 3047 | OH2 | WAT | S | 60 | 27.290 | 21.016 | 77.320 | 1.00 | 27.74 | 8 |
| ATOM | 3048 | OH2 | WAT | S | 61 | 19.809 | 49.810 | 61.716 | 1.00 | 46.14 | 8 |
| ATOM | 3049 | OH2 | WAT | S | 62 | 30.843 | 18.035 | 41.441 | 1.00 | 42.23 | 8 |
| ATOM | 3050 | OH2 | WAT | S | 63 | 19.055 | 33.379 | 60.511 | 1.00 | 28.99 | 8 |
| ATOM | 3051 | OH2 | WAT | S | 64 | 47.925 | 33.253 | 61.470 | 1.00 | 34.93 | 8 |
| ATOM | 3052 | OH2 | WAT | S | 65 | 32.500 | 36.000 | 41.000 | 1.00 | 35.33 | 8 |
| ATOM | 3053 | OH2 | WAT | S | 66 | 27.245 | 56.551 | 44.579 | 1.00 | 34.19 | 8 |
| ATOM | 3054 | OH2 | WAT | S | 67 | 5.176 | 32.914 | 54.669 | 1.00 | 41.89 | 8 |
| ATOM | 3055 | OH2 | WAT | S | 68 | 41.159 | 51.018 | 49.348 | 1.00 | 27.31 | 8 |
| ATOM | 3056 | OH2 | WAT | S | 69 | 12.869 | 50.298 | 61.877 | 1.00 | 31.30 | 8 |
| ATOM | 3057 | OH2 | WAT | S | 70 | 17.499 | 12.826 | 63.854 | 1.00 | 24.91 | 8 |
| ATOM | 3058 | OH2 | WAT | S | 71 | 27.152 | 12.189 | 53.999 | 1.00 | 18.76 | 8 |
| ATOM | 3059 | OH2 | WAT | S | 72 | 25.213 | 54.809 | 67.866 | 1.00 | 61.35 | 8 |
| ATOM | 3060 | OH2 | WAT | S | 73 | 17.671 | 48.515 | 53.188 | 1.00 | 37.63 | 8 |
| ATOM | 3061 | OH2 | WAT | S | 74 | 23.765 | 60.846 | 66.579 | 1.00 | 21.81 | 8 |
| ATOM | 3062 | OH2 | WAT | S | 75 | 35.535 | 27.040 | 70.698 | 1.00 | 34.04 | 8 |
| ATOM | 3063 | OH2 | WAT | S | 76 | 26.280 | 16.065 | 76.564 | 1.00 | 32.20 | 8 |
| ATOM | 3064 | OH2 | WAT | S | 77 | 18.451 | 25.555 | 45.150 | 1.00 | 28.55 | 8 |
| ATOM | 3065 | OH2 | WAT | S | 78 | 10.446 | 61.273 | 48.633 | 1.00 | 44.74 | 8 |
| ATOM | 3066 | OH2 | WAT | S | 79 | 13.256 | 24.051 | 73.017 | 1.00 | 35.45 | 8 |
| ATOM | 3067 | OH2 | WAT | S | 80 | 23.571 | 13.292 | 69.937 | 1.00 | 49.49 | 8 |
| ATOM | 3068 | OH2 | WAT | S | 81 | 29.891 | 18.071 | 46.109 | 1.00 | 22.84 | 8 |
| ATOM | 3069 | OH2 | WAT | S | 82 | 12.886 | 42.723 | 75.807 | 1.00 | 35.31 | 8 |
| ATOM | 3070 | OH2 | WAT | S | 83 | 41.348 | 15.471 | 45.004 | 1.00 | 47.24 | 8 |
| ATOM | 3071 | OH2 | WAT | S | 84 | 13.406 | 44.647 | 71.349 | 1.00 | 49.67 | 8 |
| ATOM | 3072 | OH2 | WAT | S | 85 | 30.444 | 35.217 | 51.882 | 1.00 | 38.15 | 8 |
| ATOM | 3073 | OH2 | WAT | S | 86 | 5.217 | 40.817 | 61.244 | 1.00 | 19.51 | 8 |
| ATOM | 3074 | OH2 | WAT | S | 87 | 8.891 | 21.532 | 56.838 | 1.00 | 30.72 | 8 |
| ATOM | 3075 | OH2 | WAT | S | 88 | 41.816 | 25.022 | 72.452 | 1.00 | 22.92 | 8 |
| ATOM | 3076 | OH2 | WAT | S | 89 | 50.621 | 36.644 | 60.248 | 1.00 | 29.29 | 8 |
| ATOM | 3077 | OH2 | WAT | S | 90 | 26.008 | 34.532 | 49.627 | 1.00 | 45.42 | 8 |
| ATOM | 3078 | OH2 | WAT | S | 91 | 8.131 | 39.168 | 54.903 | 1.00 | 31.50 | 8 |
| ATOM | 3079 | OH2 | WAT | S | 92 | 16.591 | 58.091 | 57.551 | 1.00 | 34.73 | 8 |
| ATOM | 3080 | OH2 | WAT | S | 93 | 34.773 | 54.065 | 69.382 | 1.00 | 36.05 | 8 |
| ATOM | 3081 | OH2 | WAT | S | 94 | 42.105 | 31.720 | 71.257 | 1.00 | 35.49 | 8 |
| ATOM | 3082 | OH2 | WAT | S | 95 | 29.684 | 52.077 | 73.172 | 1.00 | 35.17 | 8 |
| ATOM | 3083 | OH2 | WAT | S | 96 | 26.411 | 37.426 | 38.934 | 1.00 | 41.68 | 8 |
| ATOM | 3084 | OH2 | WAT | S | 97 | 41.183 | 52.989 | 62.927 | 1.00 | 50.77 | 8 |
| ATOM | 3085 | OH2 | WAT | S | 98 | 21.167 | 6.202 | 63.102 | 1.00 | 33.36 | 8 |
| ATOM | 3086 | OH2 | WAT | S | 99 | 25.060 | 18.985 | 36.669 | 1.00 | 46.63 | 8 |
| ATOM | 3087 | OH2 | WAT | S | 100 | 37.304 | 39.027 | 73.722 | 1.00 | 25.99 | 8 |
| ATOM | 3088 | OH2 | WAT | S | 101 | 15.911 | 54.635 | 39.343 | 1.00 | 29.88 | 8 |
| ATOM | 3089 | OH2 | WAT | S | 102 | 48.730 | 25.803 | 59.572 | 1.00 | 37.97 | 8 |
| ATOM | 3090 | OH2 | WAT | S | 103 | 24.029 | 42.997 | 74.111 | 1.00 | 25.23 | 8 |
| ATOM | 3091 | OH2 | WAT | S | 104 | 42.477 | 21.773 | 46.986 | 1.00 | 49.05 | 8 |
| ATOM | 3092 | OH2 | WAT | S | 105 | 29.984 | 22.945 | 31.397 | 1.00 | 44.21 | 8 |
| ATOM | 3093 | OH2 | WAT | S | 106 | 40.850 | 36.936 | 31.885 | 1.00 | 43.26 | 8 |
| ATOM | 3094 | OH2 | WAT | S | 107 | 9.750 | 32.487 | 48.823 | 1.00 | 35.71 | 8 |
| ATOM | 3095 | OH2 | WAT | S | 108 | 7.618 | 30.171 | 58.896 | 1.00 | 40.03 | 8 |
| ATOM | 3096 | OH2 | WAT | S | 109 | 17.603 | 13.771 | 59.767 | 1.00 | 50.33 | 8 |
| ATOM | 3097 | OH2 | WAT | S | 110 | 22.590 | 8.744 | 67.501 | 1.00 | 34.81 | 8 |
| ATOM | 3098 | OH2 | WAT | S | 111 | 21.034 | 29.771 | 76.056 | 1.00 | 30.02 | 8 |
| ATOM | 3099 | OH2 | WAT | S | 112 | 24.791 | 14.674 | 50.081 | 1.00 | 51.96 | 8 |
| ATOM | 3100 | OH2 | WAT | S | 113 | 40.750 | 47.494 | 54.056 | 1.00 | 46.98 | 8 |
| ATOM | 3101 | OH2 | WAT | S | 114 | 7.708 | 42.479 | 58.027 | 1.00 | 34.08 | 8 |
| ATOM | 3102 | OH2 | WAT | S | 115 | 32.375 | 49.136 | 77.566 | 1.00 | 27.53 | 8 |

SUBSTITUTE SHEET (RULE 26)

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Figure 17-48

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3103 | OH2 | WAT | S | 116 | 5.596 | 17.009 | 64.551 | 1.00 | 39.15 | 8 |
| ATOM | 3104 | OH2 | WAT | S | 117 | 20.194 | 50.998 | 70.563 | 1.00 | 19.73 | 8 |
| ATOM | 3105 | OH2 | WAT | S | 118 | 23.853 | 64.927 | 64.164 | 1.00 | 27.16 | 8 |
| ATOM | 3106 | OH2 | WAT | S | 119 | 9.277 | 43.601 | 46.279 | 1.00 | 32.31 | 8 |
| ATOM | 3107 | OH2 | WAT | S | 120 | 15.613 | 24.398 | 46.723 | 1.00 | 55.20 | 8 |
| ATOM | 3108 | OH2 | WAT | S | 121 | 33.110 | 16.122 | 54.229 | 1.00 | 35.91 | 8 |
| ATOM | 3109 | OH2 | WAT | S | 122 | 26.772 | 34.085 | 33.852 | 1.00 | 37.49 | 8 |
| ATOM | 3110 | OH2 | WAT | S | 123 | 28.654 | 37.783 | 75.829 | 1.00 | 47.30 | 8 |
| ATOM | 3111 | OH2 | WAT | S | 124 | 49.180 | 22.653 | 59.678 | 1.00 | 37.33 | 8 |
| ATOM | 3112 | OH2 | WAT | S | 125 | 20.561 | 27.788 | 65.975 | 1.00 | 67.86 | 8 |
| ATOM | 3113 | OH2 | WAT | S | 126 | 34.251 | 13.344 | 57.366 | 1.00 | 36.18 | 8 |
| ATOM | 3114 | OH2 | WAT | S | 127 | 49.215 | 36.854 | 48.117 | 1.00 | 33.63 | 8 |
| ATOM | 3115 | OH2 | WAT | S | 128 | 45.826 | 19.588 | 41.601 | 1.00 | 44.07 | 8 |
| ATOM | 3116 | OH2 | WAT | S | 129 | 18.693 | 56.382 | 64.014 | 1.00 | 47.77 | 8 |
| ATOM | 3117 | OH2 | WAT | S | 130 | 44.181 | 24.202 | 36.963 | 1.00 | 32.70 | 8 |
| ATOM | 3118 | OH2 | WAT | S | 131 | 19.160 | 51.901 | 38.133 | 1.00 | 54.07 | 8 |
| ATOM | 3119 | OH2 | WAT | S | 132 | 16.904 | 36.558 | 48.679 | 1.00 | 42.21 | 8 |
| ATOM | 3120 | OH2 | WAT | S | 133 | 46.851 | 26.029 | 34.353 | 1.00 | 56.33 | 8 |
| ATOM | 3121 | OH2 | WAT | S | 134 | 3.925 | 41.533 | 68.647 | 1.00 | 45.99 | 8 |
| ATOM | 3122 | OH2 | WAT | S | 135 | 44.590 | 38.382 | 78.167 | 1.00 | 44.50 | 8 |
| ATOM | 3123 | OH2 | WAT | S | 136 | 6.384 | 19.317 | 71.166 | 1.00 | 28.17 | 8 |
| ATOM | 3124 | OH2 | WAT | S | 137 | 17.982 | 39.823 | 66.487 | 1.00 | 49.31 | 8 |
| ATOM | 3125 | OH2 | WAT | S | 138 | 8.317 | 22.286 | 61.863 | 1.00 | 43.42 | 8 |
| ATOM | 3126 | OH2 | WAT | S | 139 | 29.248 | 14.196 | 55.622 | 1.00 | 35.55 | 8 |
| ATOM | 3127 | OH2 | WAT | S | 140 | 30.377 | 33.180 | 80.320 | 1.00 | 43.94 | 8 |
| ATOM | 3128 | OH2 | WAT | S | 141 | 41.842 | 32.906 | 27.392 | 1.00 | 24.82 | 8 |
| ATOM | 3129 | OH2 | WAT | S | 142 | 33.971 | 3.859 | 64.002 | 1.00 | 41.93 | 8 |
| ATOM | 3130 | OH2 | WAT | S | 143 | 27.314 | 8.087 | 70.916 | 1.00 | 49.03 | 8 |
| ATOM | 3131 | OH2 | WAT | S | 144 | 4.310 | 39.006 | 64.550 | 1.00 | 32.70 | 8 |
| ATOM | 3132 | OH2 | WAT | S | 145 | 2.940 | 19.950 | 63.265 | 1.00 | 33.24 | 8 |
| ATOM | 3133 | OH2 | WAT | S | 146 | 24.134 | 47.625 | 60.121 | 1.00 | 44.24 | 8 |
| ATOM | 3134 | OH2 | WAT | S | 147 | 25.035 | 53.746 | 42.337 | 1.00 | 47.82 | 8 |
| ATOM | 3135 | OH2 | WAT | S | 148 | 32.767 | 38.897 | 49.651 | 1.00 | 21.86 | 8 |
| ATOM | 3136 | OH2 | WAT | S | 149 | 37.145 | 57.288 | 47.392 | 1.00 | 36.13 | 8 |
| ATOM | 3137 | OH2 | WAT | S | 150 | 25.171 | 18.011 | 32.273 | 1.00 | 38.04 | 8 |
| ATOM | 3138 | OH2 | WAT | S | 151 | 24.054 | 43.182 | 55.583 | 1.00 | 41.68 | 8 |
| ATOM | 3139 | OH2 | WAT | S | 152 | 27.686 | 64.936 | 52.937 | 1.00 | 60.62 | 8 |
| ATOM | 3140 | OH2 | WAT | S | 153 | 24.084 | 39.543 | 76.589 | 1.00 | 22.62 | 8 |
| ATOM | 3141 | OH2 | WAT | S | 154 | 42.110 | 10.159 | 68.662 | 1.00 | 46.98 | 8 |
| ATOM | 3142 | OH2 | WAT | S | 155 | 9.675 | 22.905 | 75.335 | 1.00 | 26.45 | 8 |
| ATOM | 3143 | OH2 | WAT | S | 156 | 4.506 | 34.799 | 52.857 | 1.00 | 33.84 | 8 |
| ATOM | 3144 | OH2 | WAT | S | 157 | 32.583 | 35.051 | 76.446 | 1.00 | 36.27 | 8 |
| ATOM | 3145 | OH2 | WAT | S | 158 | 40.341 | 58.311 | 60.390 | 1.00 | 54.69 | 8 |
| ATOM | 3146 | OH2 | WAT | S | 159 | 29.473 | 58.378 | 71.881 | 1.00 | 28.59 | 8 |
| ATOM | 3147 | OH2 | WAT | S | 160 | 11.829 | 60.543 | 56.138 | 1.00 | 37.67 | 8 |
| ATOM | 3148 | OH2 | WAT | S | 161 | 24.247 | 48.010 | 67.935 | 1.00 | 56.62 | 8 |
| ATOM | 3149 | OH2 | WAT | S | 162 | 12.851 | 33.929 | 77.503 | 1.00 | 29.88 | 8 |
| ATOM | 3150 | OH2 | WAT | S | 163 | 9.497 | 26.168 | 59.687 | 1.00 | 15.42 | 8 |
| ATOM | 3151 | OH2 | WAT | S | 164 | 27.424 | 16.480 | 38.895 | 1.00 | 36.86 | 8 |
| ATOM | 3152 | OH2 | WAT | S | 165 | 8.512 | 56.634 | 49.614 | 1.00 | 30.08 | 8 |
| ATOM | 3153 | OH2 | WAT | S | 166 | 30.721 | 13.394 | 57.919 | 1.00 | 39.47 | 8 |
| ATOM | 3154 | OH2 | WAT | S | 167 | 49.594 | 38.223 | 73.903 | 1.00 | 29.50 | 8 |
| ATOM | 3155 | OH2 | WAT | S | 168 | 41.994 | 48.023 | 74.119 | 1.00 | 38.12 | 8 |
| ATOM | 3156 | OH2 | WAT | S | 169 | 42.092 | 39.503 | 33.116 | 1.00 | 24.47 | 8 |
| ATOM | 3157 | OH2 | WAT | S | 170 | 34.547 | 12.749 | 38.054 | 1.00 | 38.65 | 8 |
| ATOM | 3158 | OH2 | WAT | S | 171 | 15.377 | 60.862 | 50.791 | 1.00 | 32.82 | 8 |
| ATOM | 3159 | OH2 | WAT | S | 172 | 31.854 | 42.110 | 62.950 | 1.00 | 42.43 | 8 |
| ATOM | 3160 | OH2 | WAT | S | 173 | 48.743 | 44.073 | 57.626 | 1.00 | 34.04 | 8 |
| ATOM | 3161 | OH2 | WAT | S | 174 | 8.723 | 50.038 | 42.232 | 1.00 | 32.87 | 8 |
| ATOM | 3162 | OH2 | WAT | S | 175 | 14.257 | 18.280 | 53.455 | 1.00 | 40.51 | 8 |
| ATOM | 3163 | OH2 | WAT | S | 176 | 31.917 | 37.509 | 53.943 | 1.00 | 40.43 | 8 |
| ATOM | 3164 | OH2 | WAT | S | 177 | 23.921 | 47.029 | 70.642 | 1.00 | 47.97 | 8 |
| ATOM | 3165 | OH2 | WAT | S | 178 | 27.974 | 47.778 | 69.949 | 1.00 | 62.12 | 8 |
| ATOM | 3166 | OH2 | WAT | S | 179 | 7.850 | 25.093 | 51.345 | 1.00 | 50.13 | 8 |
| ATOM | 3167 | OH2 | WAT | S | 180 | 22.080 | 48.840 | 66.463 | 1.00 | 53.81 | 8 |
| ATOM | 3168 | OH2 | WAT | S | 181 | 34.780 | 48.220 | 77.419 | 1.00 | 30.86 | 8 |

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Figure 17-49

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3169 | OH2 | WAT | S | 182 | 43.893 | 35.526 | 52.018 | 1.00 | 47.14 | 8 |
| ATOM | 3170 | OH2 | WAT | S | 183 | 29.166 | 21.424 | 28.950 | 1.00 | 45.08 | 8 |
| ATOM | 3171 | OH2 | WAT | S | 184 | 51.175 | 51.545 | 62.599 | 1.00 | 33.88 | 8 |
| ATOM | 3172 | OH2 | WAT | S | 185 | 18.520 | 46.208 | 42.323 | 1.00 | 50.85 | 8 |
| ATOM | 3173 | OH2 | WAT | S | 186 | 44.774 | 30.219 | 38.653 | 1.00 | 45.36 | 8 |
| ATOM | 3174 | OH2 | WAT | S | 187 | 30.770 | 9.460 | 69.837 | 1.00 | 32.44 | 8 |
| ATOM | 3175 | OH2 | WAT | S | 188 | 22.157 | 39.535 | 78.736 | 1.00 | 37.01 | 8 |
| ATOM | 3176 | OH2 | WAT | S | 189 | 11.778 | 50.526 | 68.987 | 1.00 | 41.34 | 8 |
| ATOM | 3177 | OH2 | WAT | S | 190 | 31.339 | 60.910 | 49.439 | 1.00 | 21.88 | 8 |
| ATOM | 3178 | OH2 | WAT | S | 191 | 31.165 | 14.244 | 74.907 | 1.00 | 27.47 | 8 |
| ATOM | 3179 | OH2 | WAT | S | 192 | 39.705 | 15.398 | 70.464 | 1.00 | 47.05 | 8 |
| ATOM | 3180 | OH2 | WAT | S | 193 | 3.668 | 34.304 | 72.937 | 1.00 | 39.82 | 8 |
| ATOM | 3181 | OH2 | WAT | S | 194 | 25.256 | 9.360 | 67.925 | 1.00 | 33.21 | 8 |
| ATOM | 3182 | OH2 | WAT | S | 195 | 47.575 | 17.667 | 48.773 | 1.00 | 40.79 | 8 |
| ATOM | 3183 | OH2 | WAT | S | 196 | 32.017 | 13.045 | 34.633 | 1.00 | 37.00 | 8 |
| ATOM | 3184 | OH2 | WAT | S | 197 | 35.476 | 7.006 | 64.436 | 1.00 | 49.59 | 8 |
| ATOM | 3185 | OH2 | WAT | S | 198 | 12.180 | 16.270 | 56.288 | 1.00 | 47.22 | 8 |
| ATOM | 3186 | OH2 | WAT | S | 199 | 37.133 | 21.226 | 75.963 | 1.00 | 38.59 | 8 |
| ATOM | 3187 | OH2 | WAT | S | 200 | 40.268 | 15.712 | 48.199 | 1.00 | 39.24 | 8 |
| ATOM | 3188 | OH2 | WAT | S | 201 | 25.159 | 17.768 | 46.858 | 1.00 | 49.88 | 8 |
| ATOM | 3189 | OH2 | WAT | S | 202 | 24.593 | 27.104 | 65.727 | 1.00 | 53.46 | 8 |
| ATOM | 3190 | OH2 | WAT | S | 203 | 36.741 | 20.267 | 33.858 | 1.00 | 41.90 | 8 |
| ATOM | 3191 | OH2 | WAT | S | 204 | 10.013 | 53.930 | 47.546 | 1.00 | 48.06 | 8 |
| ATOM | 3192 | OH2 | WAT | S | 205 | 22.305 | 16.731 | 54.471 | 1.00 | 27.07 | 8 |
| ATOM | 3193 | OH2 | WAT | S | 206 | 47.454 | 34.778 | 74.101 | 1.00 | 47.44 | 8 |
| ATOM | 3194 | OH2 | WAT | S | 207 | 35.189 | 55.767 | 45.193 | 1.00 | 59.49 | 8 |
| ATOM | 3195 | OH2 | WAT | S | 208 | 37.827 | 18.151 | 36.382 | 1.00 | 45.31 | 8 |
| ATOM | 3196 | OH2 | WAT | S | 209 | 6.823 | 37.405 | 51.989 | 1.00 | 58.23 | 8 |
| ATOM | 3197 | OH2 | WAT | S | 210 | 32.040 | 43.551 | 36.157 | 1.00 | 30.78 | 8 |
| ATOM | 3198 | OH2 | WAT | S | 211 | 17.038 | 52.360 | 63.283 | 1.00 | 34.08 | 8 |
| ATOM | 3199 | OH2 | WAT | S | 212 | 30.001 | 18.471 | 49.568 | 1.00 | 33.92 | 8 |
| ATOM | 3200 | OH2 | WAT | S | 213 | 23.045 | 28.615 | 33.729 | 1.00 | 44.22 | 8 |
| ATOM | 3201 | OH2 | WAT | S | 214 | 26.130 | 61.496 | 75.246 | 1.00 | 40.49 | 8 |
| ATOM | 3202 | OH2 | WAT | S | 215 | 33.881 | 32.473 | 46.604 | 1.00 | 39.35 | 8 |
| ATOM | 3203 | OH2 | WAT | S | 216 | 23.887 | 45.987 | 44.362 | 1.00 | 36.50 | 8 |
| ATOM | 3204 | OH2 | WAT | S | 217 | 6.925 | 42.281 | 65.917 | 1.00 | 34.22 | 8 |
| ATOM | 3205 | OH2 | WAT | S | 218 | 32.823 | 8.977 | 59.213 | 1.00 | 27.03 | 8 |
| END | | | | | | | | | | | |

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Figure 18-1

| | | | | Residue # | X | Y | Z | B | Segment ID |
|------|----|-----|-----|-----------|--------|--------|---------|------|------------|
| ATOM | 1 | CB | ALA | A 2 | 46.726 | 14.971 | 138.208 | 1.00 | 56.80 |
| ATOM | 2 | C | ALA | A 2 | 47.943 | 12.813 | 138.561 | 1.00 | 58.93 |
| ATOM | 3 | O | ALA | A 2 | 48.857 | 13.292 | 137.884 | 1.00 | 60.99 |
| ATOM | 4 | N | ALA | A 2 | 46.995 | 14.046 | 140.488 | 1.00 | 56.88 |
| ATOM | 5 | CA | ALA | A 2 | 46.801 | 13.697 | 139.052 | 1.00 | 59.41 |
| ATOM | 6 | N | LYS | A 3 | 47.890 | 11.525 | 138.903 | 1.00 | 53.81 |
| ATOM | 7 | CA | LYS | A 3 | 48.937 | 10.591 | 138.492 | 1.00 | 53.62 |
| ATOM | 8 | CB | LYS | A 3 | 48.736 | 9.229 | 139.156 | 1.00 | 50.26 |
| ATOM | 9 | CG | LYS | A 3 | 48.917 | 9.279 | 140.665 | 1.00 | 56.64 |
| ATOM | 10 | CD | LYS | A 3 | 48.950 | 7.891 | 141.285 | 1.00 | 57.18 |
| ATOM | 11 | CE | LYS | A 3 | 49.160 | 7.964 | 142.796 | 1.00 | 56.74 |
| ATOM | 12 | NZ | LYS | A 3 | 50.423 | 8.663 | 143.165 | 1.00 | 54.86 |
| ATOM | 13 | C | LYS | A 3 | 49.063 | 10.430 | 136.986 | 1.00 | 49.95 |
| ATOM | 14 | O | LYS | A 3 | 48.088 | 10.562 | 136.248 | 1.00 | 44.34 |
| ATOM | 15 | N | VAL | A 4 | 50.287 | 10.147 | 136.550 | 1.00 | 46.01 |
| ATOM | 16 | CA | VAL | A 4 | 50.609 | 9.985 | 135.142 | 1.00 | 42.48 |
| ATOM | 17 | CB | VAL | A 4 | 51.901 | 10.755 | 134.809 | 1.00 | 43.42 |
| ATOM | 18 | CG1 | VAL | A 4 | 52.179 | 10.713 | 133.307 | 1.00 | 39.20 |
| ATOM | 19 | CG2 | VAL | A 4 | 51.773 | 12.186 | 135.310 | 1.00 | 39.34 |
| ATOM | 20 | C | VAL | A 4 | 50.787 | 8.510 | 134.806 | 1.00 | 38.41 |
| ATOM | 21 | O | VAL | A 4 | 51.659 | 7.839 | 135.351 | 1.00 | 37.08 |
| ATOM | 22 | N | LYS | A 5 | 49.959 | 8.011 | 133.899 | 1.00 | 37.79 |
| ATOM | 23 | CA | LYS | A 5 | 50.016 | 6.610 | 133.515 | 1.00 | 38.17 |
| ATOM | 24 | CB | LYS | A 5 | 48.700 | 5.915 | 133.887 | 1.00 | 38.40 |
| ATOM | 25 | CG | LYS | A 5 | 48.411 | 5.803 | 135.385 | 1.00 | 42.84 |
| ATOM | 26 | CD | LYS | A 5 | 49.384 | 4.855 | 136.070 | 1.00 | 44.10 |
| ATOM | 27 | CE | LYS | A 5 | 49.017 | 4.632 | 137.534 | 1.00 | 45.97 |
| ATOM | 28 | NZ | LYS | A 5 | 49.045 | 5.894 | 138.322 | 1.00 | 51.78 |
| ATOM | 29 | C | LYS | A 5 | 50.275 | 6.392 | 132.030 | 1.00 | 38.31 |
| ATOM | 30 | O | LYS | A 5 | 49.992 | 7.253 | 131.201 | 1.00 | 38.13 |
| ATOM | 31 | N | LEU | A 6 | 50.817 | 5.220 | 131.717 | 1.00 | 35.05 |
| ATOM | 32 | CA | LEU | A 6 | 51.082 | 4.818 | 130.346 | 1.00 | 31.46 |
| ATOM | 33 | CB | LEU | A 6 | 52.582 | 4.592 | 130.133 | 1.00 | 28.46 |
| ATOM | 34 | CG | LEU | A 6 | 53.094 | 4.256 | 128.720 | 1.00 | 30.91 |
| ATOM | 35 | CD1 | LEU | A 6 | 52.618 | 2.884 | 128.295 | 1.00 | 33.05 |
| ATOM | 36 | CD2 | LEU | A 6 | 52.630 | 5.312 | 127.744 | 1.00 | 21.96 |
| ATOM | 37 | C | LEU | A 6 | 50.307 | 3.512 | 130.164 | 1.00 | 30.50 |
| ATOM | 38 | O | LEU | A 6 | 50.453 | 2.581 | 130.955 | 1.00 | 32.82 |
| ATOM | 39 | N | ILE | A 7 | 49.459 | 3.456 | 129.145 | 1.00 | 26.94 |
| ATOM | 40 | CA | ILE | A 7 | 48.676 | 2.255 | 128.893 | 1.00 | 28.29 |
| ATOM | 41 | CB | ILE | A 7 | 47.218 | 2.598 | 128.493 | 1.00 | 28.94 |
| ATOM | 42 | CG2 | ILE | A 7 | 46.499 | 1.343 | 128.041 | 1.00 | 32.57 |
| ATOM | 43 | CG1 | ILE | A 7 | 46.447 | 3.172 | 129.688 | 1.00 | 36.59 |
| ATOM | 44 | CD1 | ILE | A 7 | 46.979 | 4.468 | 130.236 | 1.00 | 46.80 |
| ATOM | 45 | C | ILE | A 7 | 49.341 | 1.470 | 127.770 | 1.00 | 31.09 |
| ATOM | 46 | O | ILE | A 7 | 49.600 | 2.009 | 126.695 | 1.00 | 27.65 |
| ATOM | 47 | N | GLU | A 8 | 49.638 | 0.201 | 128.029 | 1.00 | 27.30 |
| ATOM | 48 | CA | GLU | A 8 | 50.277 | -0.614 | 127.016 | 1.00 | 25.50 |
| ATOM | 49 | C | GLY | A 8 | 50.578 | -2.024 | 127.480 | 1.00 | 30.66 |
| ATOM | 50 | O | GLY | A 8 | 50.224 | -2.421 | 128.592 | 1.00 | 30.02 |
| ATOM | 51 | N | THR | A 9 | 51.238 | -2.777 | 126.611 | 1.00 | 28.94 |
| ATOM | 52 | CA | THR | A 9 | 51.614 | -4.156 | 126.877 | 1.00 | 33.63 |
| ATOM | 53 | CB | THR | A 9 | 50.393 | -5.083 | 126.857 | 1.00 | 36.19 |
| ATOM | 54 | OG1 | THR | A 9 | 50.827 | -6.441 | 126.992 | 1.00 | 34.87 |
| ATOM | 55 | CG2 | THR | A 9 | 49.633 | -4.931 | 125.548 | 1.00 | 36.49 |
| ATOM | 56 | C | THR | A 9 | 52.567 | -4.637 | 125.794 | 1.00 | 34.83 |
| ATOM | 57 | O | THR | A 9 | 52.545 | -4.133 | 124.677 | 1.00 | 36.91 |
| ATOM | 58 | N | LEU | A 10 | 53.407 | -5.609 | 126.129 | 1.00 | 39.15 |
| ATOM | 59 | CA | LEU | A 10 | 54.345 | -6.167 | 125.164 | 1.00 | 40.21 |
| ATOM | 60 | CB | LEU | A 10 | 55.402 | -7.009 | 125.881 | 1.00 | 42.40 |
| ATOM | 61 | CG | LEU | A 10 | 56.482 | -6.282 | 126.687 | 1.00 | 42.29 |
| ATOM | 62 | CD1 | LEU | A 10 | 55.870 | -5.293 | 127.647 | 1.00 | 42.92 |
| ATOM | 63 | CD2 | LEU | A 10 | 57.319 | -7.306 | 127.424 | 1.00 | 40.29 |
| ATOM | 64 | C | LEU | A 10 | 53.591 | -7.039 | 124.159 | 1.00 | 41.70 |
| ATOM | 65 | O | LEU | A 10 | 54.055 | -7.266 | 123.044 | 1.00 | 37.13 |
| ATOM | 66 | N | ASP | A 11 | 52.419 | -7.519 | 124.557 | 1.00 | 47.28 |

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Figure 18-2

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|---------|------|-------|
| ATOM | 67 | CA | ASP | A | 11 | 51.617 | -8.369 | 123.683 | 1.00 | 53.30 |
| ATOM | 68 | CB | ASP | A | 11 | 50.230 | -8.608 | 124.287 | 1.00 | 52.35 |
| ATOM | 69 | CG | ASP | A | 11 | 50.295 | -9.331 | 125.610 | 1.00 | 53.33 |
| ATOM | 70 | OD1 | ASP | A | 11 | 51.004 | -10.358 | 125.685 | 1.00 | 52.21 |
| ATOM | 71 | OD2 | ASP | A | 11 | 49.630 | -8.883 | 126.567 | 1.00 | 58.48 |
| ATOM | 72 | C | ASP | A | 11 | 51.459 | -7.840 | 122.257 | 1.00 | 53.33 |
| ATOM | 73 | O | ASP | A | 11 | 51.360 | -8.626 | 121.311 | 1.00 | 54.31 |
| ATOM | 74 | N | TYR | A | 12 | 51.424 | -6.521 | 122.092 | 1.00 | 51.92 |
| ATOM | 75 | CA | TYR | A | 12 | 51.275 | -5.970 | 120.749 | 1.00 | 51.41 |
| ATOM | 76 | CB | TYR | A | 12 | 51.328 | -4.437 | 120.755 | 1.00 | 49.05 |
| ATOM | 77 | CG | TYR | A | 12 | 50.164 | -3.729 | 121.421 | 1.00 | 45.48 |
| ATOM | 78 | CD1 | TYR | A | 12 | 50.296 | -3.157 | 122.686 | 1.00 | 47.08 |
| ATOM | 79 | CE1 | TYR | A | 12 | 49.252 | -2.430 | 123.263 | 1.00 | 47.53 |
| ATOM | 80 | CD2 | TYR | A | 12 | 48.952 | -3.565 | 120.749 | 1.00 | 43.77 |
| ATOM | 81 | CE2 | TYR | A | 12 | 47.906 | -2.847 | 121.310 | 1.00 | 44.16 |
| ATOM | 82 | CZ | TYR | A | 12 | 48.061 | -2.279 | 122.566 | 1.00 | 48.67 |
| ATOM | 83 | OH | TYR | A | 12 | 47.030 | -1.548 | 123.116 | 1.00 | 48.65 |
| ATOM | 84 | C | TYR | A | 12 | 52.367 | -6.503 | 119.816 | 1.00 | 50.01 |
| ATOM | 85 | O | TYR | A | 12 | 52.197 | -6.525 | 118.596 | 1.00 | 45.56 |
| ATOM | 86 | N | GLY | A | 13 | 53.484 | -6.931 | 120.396 | 1.00 | 48.72 |
| ATOM | 87 | CA | GLY | A | 13 | 54.574 | -7.458 | 119.599 | 1.00 | 50.56 |
| ATOM | 88 | C | GLY | A | 13 | 54.196 | -8.727 | 118.857 | 1.00 | 53.32 |
| ATOM | 89 | O | GLY | A | 13 | 54.931 | -9.184 | 117.982 | 1.00 | 52.64 |
| ATOM | 90 | N | LYS | A | 14 | 53.045 | -9.294 | 119.207 | 1.00 | 53.37 |
| ATOM | 91 | CA | LYS | A | 14 | 52.555 | -10.518 | 118.579 | 1.00 | 54.56 |
| ATOM | 92 | CB | LYS | A | 14 | 52.022 | -11.475 | 119.653 | 1.00 | 58.02 |
| ATOM | 93 | CG | LYS | A | 14 | 53.086 | -12.062 | 120.591 | 1.00 | 62.81 |
| ATOM | 94 | CD | LYS | A | 14 | 53.934 | -13.154 | 119.918 | 1.00 | 61.61 |
| ATOM | 95 | CE | LYS | A | 14 | 54.747 | -12.638 | 118.734 | 1.00 | 61.77 |
| ATOM | 96 | NZ | LYS | A | 14 | 55.514 | -13.713 | 118.045 | 1.00 | 58.35 |
| ATOM | 97 | C | LYS | A | 14 | 51.455 | -10.231 | 117.559 | 1.00 | 52.03 |
| ATOM | 98 | O | LYS | A | 14 | 50.911 | -11.145 | 116.942 | 1.00 | 51.71 |
| ATOM | 99 | N | TYR | A | 15 | 51.143 | -8.955 | 117.372 | 1.00 | 46.92 |
| ATOM | 100 | CA | TYR | A | 15 | 50.091 | -8.563 | 116.449 | 1.00 | 47.99 |
| ATOM | 101 | CB | TYR | A | 15 | 48.959 | -7.915 | 117.253 | 1.00 | 50.40 |
| ATOM | 102 | CG | TYR | A | 15 | 48.456 | -8.793 | 118.386 | 1.00 | 53.01 |
| ATOM | 103 | CD1 | TYR | A | 15 | 48.166 | -8.255 | 119.637 | 1.00 | 52.10 |
| ATOM | 104 | CE1 | TYR | A | 15 | 47.722 | -9.053 | 120.685 | 1.00 | 51.72 |
| ATOM | 105 | CD2 | TYR | A | 15 | 48.283 | -10.166 | 118.208 | 1.00 | 54.67 |
| ATOM | 106 | CE2 | TYR | A | 15 | 47.838 | -10.976 | 119.250 | 1.00 | 55.69 |
| ATOM | 107 | CZ | TYR | A | 15 | 47.561 | -10.412 | 120.485 | 1.00 | 54.18 |
| ATOM | 108 | OH | TYR | A | 15 | 47.130 | -11.208 | 121.520 | 1.00 | 55.42 |
| ATOM | 109 | C | TYR | A | 15 | 50.592 | -7.617 | 115.353 | 1.00 | 46.20 |
| ATOM | 110 | O | TYR | A | 15 | 49.933 | -6.635 | 115.018 | 1.00 | 43.72 |
| ATOM | 111 | N | ARG | A | 16 | 51.758 | -7.924 | 114.791 | 1.00 | 46.29 |
| ATOM | 112 | CA | ARG | A | 16 | 52.347 | -7.109 | 113.727 | 1.00 | 45.66 |
| ATOM | 113 | CB | ARG | A | 16 | 53.779 | -7.545 | 113.441 | 1.00 | 50.56 |
| ATOM | 114 | CG | ARG | A | 16 | 54.677 | -7.698 | 114.636 | 1.00 | 56.90 |
| ATOM | 115 | CD | ARG | A | 16 | 54.992 | -6.388 | 115.315 | 1.00 | 60.72 |
| ATOM | 116 | NE | ARG | A | 16 | 56.021 | -6.602 | 116.328 | 1.00 | 66.70 |
| ATOM | 117 | CZ | ARG | A | 16 | 57.211 | -7.141 | 116.070 | 1.00 | 66.68 |
| ATOM | 118 | NH1 | ARG | A | 16 | 57.520 | -7.519 | 114.834 | 1.00 | 65.68 |
| ATOM | 119 | NH2 | ARG | A | 16 | 58.093 | -7.314 | 117.046 | 1.00 | 66.33 |
| ATOM | 120 | C | ARG | A | 16 | 51.573 | -7.298 | 112.429 | 1.00 | 44.20 |
| ATOM | 121 | O | ARG | A | 16 | 50.871 | -8.293 | 112.254 | 1.00 | 43.41 |
| ATOM | 122 | N | TYR | A | 17 | 51.715 | -6.346 | 111.514 | 1.00 | 39.23 |
| ATOM | 123 | CA | TYR | A | 17 | 51.067 | -6.453 | 110.215 | 1.00 | 38.71 |
| ATOM | 124 | CB | TYR | A | 17 | 50.913 | -5.072 | 109.565 | 1.00 | 33.83 |
| ATOM | 125 | CG | TYR | A | 17 | 49.744 | -4.255 | 110.084 | 1.00 | 27.35 |
| ATOM | 126 | CD1 | TYR | A | 17 | 49.598 | -3.982 | 111.443 | 1.00 | 27.25 |
| ATOM | 127 | CE1 | TYR | A | 17 | 48.540 | -3.184 | 111.909 | 1.00 | 27.16 |
| ATOM | 128 | CD2 | TYR | A | 17 | 48.807 | -3.720 | 109.204 | 1.00 | 25.78 |
| ATOM | 129 | CE2 | TYR | A | 17 | 47.752 | -2.925 | 109.656 | 1.00 | 26.34 |
| ATOM | 130 | CZ | TYR | A | 17 | 47.626 | -2.659 | 111.009 | 1.00 | 27.28 |
| ATOM | 131 | OH | TYR | A | 17 | 46.602 | -1.842 | 111.450 | 1.00 | 22.04 |
| ATOM | 132 | C | TYR | A | 17 | 51.972 | -7.350 | 109.368 | 1.00 | 41.52 |

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Figure 18-3

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|---------|------|-------|
| ATOM | 133 | O | TYR | A | 17 | 53.150 | -7.525 | 109.683 | 1.00 | 35.63 |
| ATOM | 134 | N | PRO | A | 18 | 51.440 | -7.925 | 108.278 | 1.00 | 46.68 |
| ATOM | 135 | CD | PRO | A | 18 | 50.076 | -7.765 | 107.755 | 1.00 | 47.16 |
| ATOM | 136 | CA | PRO | A | 18 | 52.205 | -8.812 | 107.392 | 1.00 | 48.87 |
| ATOM | 137 | CB | PRO | A | 18 | 51.213 | -9.091 | 106.262 | 1.00 | 48.14 |
| ATOM | 138 | CG | PRO | A | 18 | 50.343 | -7.837 | 106.274 | 1.00 | 55.13 |
| ATOM | 139 | C | PRO | A | 18 | 53.556 | -8.303 | 106.885 | 1.00 | 49.67 |
| ATOM | 140 | O | PRO | A | 18 | 53.788 | -7.101 | 106.766 | 1.00 | 49.33 |
| ATOM | 141 | N | LYS | A | 19 | 54.432 | -9.261 | 106.592 | 1.00 | 53.22 |
| ATOM | 142 | CA | LYS | A | 19 | 55.800 | -9.044 | 106.114 | 1.00 | 57.00 |
| ATOM | 143 | CB | LYS | A | 19 | 56.223 | -10.242 | 105.252 | 1.00 | 62.34 |
| ATOM | 144 | CG | LYS | A | 19 | 55.069 | -10.929 | 104.537 | 1.00 | 67.94 |
| ATOM | 145 | CD | LYS | A | 19 | 54.239 | -9.963 | 103.714 | 1.00 | 70.76 |
| ATOM | 146 | CE | LYS | A | 19 | 53.004 | -10.653 | 103.162 | 1.00 | 73.70 |
| ATOM | 147 | NZ | LYS | A | 19 | 52.116 | -9.701 | 102.442 | 1.00 | 79.01 |
| ATOM | 148 | C | LYS | A | 19 | 56.229 | -7.757 | 105.405 | 1.00 | 55.93 |
| ATOM | 149 | O | LYS | A | 19 | 57.230 | -7.150 | 105.796 | 1.00 | 59.86 |
| ATOM | 150 | N | ASN | A | 20 | 55.515 | -7.338 | 104.367 | 1.00 | 49.62 |
| ATOM | 151 | CA | ASN | A | 20 | 55.925 | -6.130 | 103.652 | 1.00 | 50.02 |
| ATOM | 152 | CB | ASN | A | 20 | 55.829 | -6.359 | 102.143 | 1.00 | 50.62 |
| ATOM | 153 | CG | ASN | A | 20 | 56.729 | -7.487 | 101.670 | 1.00 | 51.26 |
| ATOM | 154 | OD1 | ASN | A | 20 | 57.948 | -7.437 | 101.843 | 1.00 | 46.88 |
| ATOM | 155 | ND2 | ASN | A | 20 | 56.130 | -8.513 | 101.074 | 1.00 | 50.85 |
| ATOM | 156 | C | ASN | A | 20 | 55.167 | -4.862 | 104.023 | 1.00 | 45.50 |
| ATOM | 157 | O | ASN | A | 20 | 55.481 | -3.778 | 103.533 | 1.00 | 45.35 |
| ATOM | 158 | N | HIS | A | 21 | 54.182 | -4.997 | 104.899 | 1.00 | 37.46 |
| ATOM | 159 | CA | HIS | A | 21 | 53.374 | -3.863 | 105.321 | 1.00 | 32.39 |
| ATOM | 160 | CB | HIS | A | 21 | 52.198 | -4.355 | 106.162 | 1.00 | 29.34 |
| ATOM | 161 | CG | HIS | A | 21 | 51.118 | -3.339 | 106.348 | 1.00 | 30.50 |
| ATOM | 162 | CD2 | HIS | A | 21 | 50.999 | -2.314 | 107.223 | 1.00 | 22.88 |
| ATOM | 163 | ND1 | HIS | A | 21 | 49.993 | -3.298 | 105.552 | 1.00 | 30.15 |
| ATOM | 164 | CE1 | HIS | A | 21 | 49.226 | -2.293 | 105.933 | 1.00 | 30.96 |
| ATOM | 165 | NE2 | HIS | A | 21 | 49.814 | -1.680 | 106.945 | 1.00 | 36.41 |
| ATOM | 166 | C | HIS | A | 21 | 54.194 | -2.879 | 106.155 | 1.00 | 29.18 |
| ATOM | 167 | O | HIS | A | 21 | 55.030 | -3.279 | 106.963 | 1.00 | 26.92 |
| ATOM | 168 | N | PRO | A | 22 | 53.965 | -1.572 | 105.969 | 1.00 | 31.12 |
| ATOM | 169 | CD | PRO | A | 22 | 53.027 | -0.912 | 105.043 | 1.00 | 29.46 |
| ATOM | 170 | CA | PRO | A | 22 | 54.702 | -0.567 | 106.739 | 1.00 | 29.27 |
| ATOM | 171 | CB | PRO | A | 22 | 54.012 | 0.732 | 106.326 | 1.00 | 26.00 |
| ATOM | 172 | CG | PRO | A | 22 | 53.670 | 0.434 | 104.875 | 1.00 | 31.52 |
| ATOM | 173 | C | PRO | A | 22 | 54.624 | -0.822 | 108.253 | 1.00 | 29.96 |
| ATOM | 174 | O | PRO | A | 22 | 55.575 | -0.538 | 108.981 | 1.00 | 27.47 |
| ATOM | 175 | N | LEU | A | 23 | 53.501 | -1.371 | 108.715 | 1.00 | 26.64 |
| ATOM | 176 | CA | LEU | A | 23 | 53.309 | -1.644 | 110.144 | 1.00 | 30.44 |
| ATOM | 177 | CB | LEU | A | 23 | 51.833 | -1.428 | 110.515 | 1.00 | 24.09 |
| ATOM | 178 | CG | LEU | A | 23 | 51.356 | 0.029 | 110.479 | 1.00 | 25.30 |
| ATOM | 179 | CD1 | LEU | A | 23 | 49.836 | 0.103 | 110.668 | 1.00 | 17.72 |
| ATOM | 180 | CD2 | LEU | A | 23 | 52.086 | 0.816 | 111.574 | 1.00 | 24.15 |
| ATOM | 181 | C | LEU | A | 23 | 53.775 | -3.015 | 110.662 | 1.00 | 31.64 |
| ATOM | 182 | O | LEU | A | 23 | 53.252 | -3.512 | 111.667 | 1.00 | 31.00 |
| ATOM | 183 | N | LYS | A | 24 | 54.753 | -3.636 | 110.012 | 1.00 | 28.25 |
| ATOM | 184 | CA | LYS | A | 24 | 55.200 | -4.929 | 110.513 | 1.00 | 30.90 |
| ATOM | 185 | CB | LYS | A | 24 | 55.718 | -5.810 | 109.372 | 1.00 | 36.59 |
| ATOM | 186 | CG | LYS | A | 24 | 57.178 | -5.650 | 108.982 | 1.00 | 40.77 |
| ATOM | 187 | CD | LYS | A | 24 | 57.546 | -4.259 | 108.535 | 1.00 | 44.61 |
| ATOM | 188 | CE | LYS | A | 24 | 58.858 | -4.303 | 107.755 | 1.00 | 50.44 |
| ATOM | 189 | NZ | LYS | A | 24 | 59.959 | -4.990 | 108.487 | 1.00 | 51.30 |
| ATOM | 190 | C | LYS | A | 24 | 56.282 | -4.736 | 111.581 | 1.00 | 32.57 |
| ATOM | 191 | O | LYS | A | 24 | 56.695 | -5.683 | 112.245 | 1.00 | 29.83 |
| ATOM | 192 | N | ILE | A | 25 | 56.729 | -3.497 | 111.750 | 1.00 | 27.06 |
| ATOM | 193 | CA | ILE | A | 25 | 57.755 | -3.200 | 112.739 | 1.00 | 30.45 |
| ATOM | 194 | CB | ILE | A | 25 | 58.416 | -1.822 | 112.499 | 1.00 | 33.37 |
| ATOM | 195 | CG2 | ILE | A | 25 | 59.056 | -1.757 | 111.120 | 1.00 | 33.22 |
| ATOM | 196 | CG1 | ILE | A | 25 | 57.361 | -0.722 | 112.662 | 1.00 | 30.45 |
| ATOM | 197 | CD1 | ILE | A | 25 | 57.930 | 0.689 | 112.700 | 1.00 | 33.12 |
| ATOM | 198 | C | ILE | A | 25 | 57.156 | -3.129 | 114.141 | 1.00 | 32.10 |

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Figure 18-4

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|
| ATOM | 199 | O | ILE | A | 25 | 55.967 | -2.851 | 114.310 | 1.00 | 28.15 |
| ATOM | 200 | N | PRO | A | 26 | 57.979 | -3.382 | 115.168 | 1.00 | 31.64 |
| ATOM | 201 | CD | PRO | A | 26 | 59.395 | -3.768 | 115.139 | 1.00 | 31.11 |
| ATOM | 202 | CA | PRO | A | 26 | 57.507 | -3.322 | 116.556 | 1.00 | 31.04 |
| ATOM | 203 | CB | PRO | A | 26 | 58.709 | -3.840 | 117.347 | 1.00 | 32.41 |
| ATOM | 204 | CG | PRO | A | 26 | 59.454 | -4.691 | 116.324 | 1.00 | 39.33 |
| ATOM | 205 | C | PRO | A | 26 | 57.265 | -1.840 | 116.827 | 1.00 | 28.42 |
| ATOM | 206 | O | PRO | A | 26 | 58.001 | -0.994 | 116.315 | 1.00 | 22.23 |
| ATOM | 207 | N | ARG | A | 27 | 56.251 | -1.514 | 117.614 | 1.00 | 24.16 |
| ATOM | 208 | CA | ARG | A | 27 | 55.977 | -0.116 | 117.899 | 1.00 | 28.53 |
| ATOM | 209 | CB | ARG | A | 27 | 54.787 | 0.358 | 117.048 | 1.00 | 29.77 |
| ATOM | 210 | CG | ARG | A | 27 | 55.075 | 0.191 | 115.554 | 1.00 | 29.64 |
| ATOM | 211 | CD | ARG | A | 27 | 53.918 | 0.538 | 114.620 | 1.00 | 26.61 |
| ATOM | 212 | NE | ARG | A | 27 | 53.622 | 1.965 | 114.517 | 1.00 | 28.52 |
| ATOM | 213 | CZ | ARG | A | 27 | 52.649 | 2.591 | 115.173 | 1.00 | 29.70 |
| ATOM | 214 | NH1 | ARG | A | 27 | 51.857 | 1.924 | 115.999 | 1.00 | 30.17 |
| ATOM | 215 | NH2 | ARG | A | 27 | 52.451 | 3.889 | 114.983 | 1.00 | 23.25 |
| ATOM | 216 | C | ARG | A | 27 | 55.746 | 0.114 | 119.387 | 1.00 | 30.71 |
| ATOM | 217 | O | ARG | A | 27 | 56.679 | 0.490 | 120.113 | 1.00 | 24.60 |
| ATOM | 218 | N | VAL | A | 28 | 54.529 | -0.117 | 119.863 | 1.00 | 23.51 |
| ATOM | 219 | CA | VAL | A | 28 | 54.282 | 0.093 | 121.282 | 1.00 | 29.33 |
| ATOM | 220 | CB | VAL | A | 28 | 52.800 | -0.124 | 121.635 | 1.00 | 34.56 |
| ATOM | 221 | CG1 | VAL | A | 28 | 52.599 | 0.002 | 123.142 | 1.00 | 32.42 |
| ATOM | 222 | CG2 | VAL | A | 28 | 51.947 | 0.908 | 120.903 | 1.00 | 33.77 |
| ATOM | 223 | C | VAL | A | 28 | 55.158 | -0.816 | 122.145 | 1.00 | 29.75 |
| ATOM | 224 | O | VAL | A | 28 | 55.673 | -0.394 | 123.182 | 1.00 | 32.49 |
| ATOM | 225 | N | SER | A | 29 | 55.341 | -2.059 | 121.718 | 1.00 | 26.09 |
| ATOM | 226 | CA | SER | A | 29 | 56.162 | -2.982 | 122.483 | 1.00 | 31.39 |
| ATOM | 227 | CB | SER | A | 29 | 56.058 | -4.399 | 121.905 | 1.00 | 26.92 |
| ATOM | 228 | OG | SER | A | 29 | 56.562 | -4.464 | 120.579 | 1.00 | 33.85 |
| ATOM | 229 | C | SER | A | 29 | 57.609 | -2.482 | 122.453 | 1.00 | 34.77 |
| ATOM | 230 | O | SER | A | 29 | 58.378 | -2.718 | 123.391 | 1.00 | 29.39 |
| ATOM | 231 | N | LEU | A | 30 | 57.967 | -1.778 | 121.380 | 1.00 | 31.20 |
| ATOM | 232 | CA | LEU | A | 30 | 59.317 | -1.234 | 121.240 | 1.00 | 32.03 |
| ATOM | 233 | CB | LEU | A | 30 | 59.554 | -0.668 | 119.829 | 1.00 | 30.86 |
| ATOM | 234 | CG | LEU | A | 30 | 61.008 | -0.550 | 119.333 | 1.00 | 33.22 |
| ATOM | 235 | CD1 | LEU | A | 30 | 61.066 | 0.484 | 118.224 | 1.00 | 28.76 |
| ATOM | 236 | CD2 | LEU | A | 30 | 61.948 | -0.135 | 120.441 | 1.00 | 35.11 |
| ATOM | 237 | C | LEU | A | 30 | 59.423 | -0.089 | 122.236 | 1.00 | 30.29 |
| ATOM | 238 | O | LEU | A | 30 | 60.397 | 0.019 | 122.984 | 1.00 | 27.69 |
| ATOM | 239 | N | LEU | A | 31 | 58.408 | 0.769 | 122.232 | 1.00 | 27.38 |
| ATOM | 240 | CA | LEU | A | 31 | 58.372 | 1.915 | 123.126 | 1.00 | 24.94 |
| ATOM | 241 | CB | LEU | A | 31 | 57.008 | 2.596 | 123.042 | 1.00 | 24.92 |
| ATOM | 242 | CG | LEU | A | 31 | 56.918 | 4.069 | 123.460 | 1.00 | 30.49 |
| ATOM | 243 | CD1 | LEU | A | 31 | 55.492 | 4.390 | 123.881 | 1.00 | 24.71 |
| ATOM | 244 | CD2 | LEU | A | 31 | 57.851 | 4.355 | 124.603 | 1.00 | 27.32 |
| ATOM | 245 | C | LEU | A | 31 | 58.610 | 1.429 | 124.564 | 1.00 | 28.18 |
| ATOM | 246 | O | LEU | A | 31 | 59.489 | 1.928 | 125.263 | 1.00 | 33.64 |
| ATOM | 247 | N | LEU | A | 32 | 57.831 | 0.445 | 125.000 | 1.00 | 30.17 |
| ATOM | 248 | CA | LEU | A | 32 | 57.965 | -0.084 | 126.357 | 1.00 | 30.59 |
| ATOM | 249 | CB | LEU | A | 32 | 56.944 | -1.206 | 126.601 | 1.00 | 30.55 |
| ATOM | 250 | CG | LEU | A | 32 | 55.458 | -0.879 | 126.402 | 1.00 | 29.50 |
| ATOM | 251 | CD1 | LEU | A | 32 | 54.611 | -2.107 | 126.727 | 1.00 | 28.31 |
| ATOM | 252 | CD2 | LEU | A | 32 | 55.058 | 0.273 | 127.287 | 1.00 | 31.92 |
| ATOM | 253 | C | LEU | A | 32 | 59.376 | -0.597 | 126.657 | 1.00 | 33.56 |
| ATOM | 254 | O | LEU | A | 32 | 59.961 | -0.243 | 127.682 | 1.00 | 36.51 |
| ATOM | 255 | N | ARG | A | 33 | 59.926 | -1.429 | 125.777 | 1.00 | 29.75 |
| ATOM | 256 | CA | ARG | A | 33 | 61.271 | -1.953 | 125.999 | 1.00 | 33.49 |
| ATOM | 257 | CB | ARG | A | 33 | 61.630 | -3.003 | 124.945 | 1.00 | 39.50 |
| ATOM | 258 | CG | ARG | A | 33 | 60.814 | -4.283 | 125.024 | 1.00 | 44.40 |
| ATOM | 259 | CD | ARG | A | 33 | 61.237 | -5.256 | 123.933 | 1.00 | 53.68 |
| ATOM | 260 | NE | ARG | A | 33 | 60.515 | -6.522 | 124.007 | 1.00 | 56.66 |
| ATOM | 261 | CZ | ARG | A | 33 | 60.611 | -7.384 | 125.014 | 1.00 | 58.73 |
| ATOM | 262 | NH1 | ARG | A | 33 | 61.402 | -7.121 | 126.045 | 1.00 | 59.32 |
| ATOM | 263 | NH2 | ARG | A | 33 | 59.911 | -8.511 | 124.991 | 1.00 | 57.91 |
| ATOM | 264 | C | ARG | A | 33 | 62.314 | -0.845 | 125.978 | 1.00 | 31.45 |

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Figure 18-5

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|
| ATOM | 265 | O | ARG | A | 33 | 63.288 | -0.885 | 126.722 | 1.00 | 26.49 |
| ATOM | 266 | N | PHE | A | 34 | 62.103 | 0.146 | 125.123 | 1.00 | 32.42 |
| ATOM | 267 | CA | PHE | A | 34 | 63.042 | 1.253 | 125.000 | 1.00 | 33.37 |
| ATOM | 268 | CB | PHE | A | 34 | 62.617 | 2.180 | 123.858 | 1.00 | 31.68 |
| ATOM | 269 | CG | PHE | A | 34 | 63.653 | 3.202 | 123.486 | 1.00 | 29.05 |
| ATOM | 270 | CD1 | PHE | A | 34 | 64.825 | 2.819 | 122.838 | 1.00 | 29.21 |
| ATOM | 271 | CD2 | PHE | A | 34 | 63.458 | 4.546 | 123.781 | 1.00 | 28.25 |
| ATOM | 272 | CE1 | PHE | A | 34 | 65.793 | 3.763 | 122.484 | 1.00 | 29.35 |
| ATOM | 273 | CE2 | PHE | A | 34 | 64.416 | 5.501 | 123.435 | 1.00 | 32.67 |
| ATOM | 274 | CZ | PHE | A | 34 | 65.589 | 5.108 | 122.783 | 1.00 | 29.08 |
| ATOM | 275 | C | PHE | A | 34 | 63.083 | 2.042 | 126.305 | 1.00 | 33.47 |
| ATOM | 276 | O | PHE | A | 34 | 64.155 | 2.294 | 126.852 | 1.00 | 27.49 |
| ATOM | 277 | N | LYS | A | 35 | 61.912 | 2.432 | 126.802 | 1.00 | 29.34 |
| ATOM | 278 | CA | LYS | A | 35 | 61.848 | 3.191 | 128.042 | 1.00 | 31.48 |
| ATOM | 279 | CB | LYS | A | 35 | 60.406 | 3.576 | 128.374 | 1.00 | 30.82 |
| ATOM | 280 | CG | LYS | A | 35 | 59.803 | 4.552 | 127.395 | 1.00 | 32.98 |
| ATOM | 281 | CD | LYS | A | 35 | 58.404 | 4.974 | 127.790 | 1.00 | 40.93 |
| ATOM | 282 | CE | LYS | A | 35 | 57.410 | 3.827 | 127.688 | 1.00 | 44.56 |
| ATOM | 283 | NZ | LYS | A | 35 | 57.754 | 2.656 | 128.548 | 1.00 | 55.10 |
| ATOM | 284 | C | LYS | A | 35 | 62.443 | 2.387 | 129.183 | 1.00 | 34.47 |
| ATOM | 285 | O | LYS | A | 35 | 63.136 | 2.933 | 130.043 | 1.00 | 32.01 |
| ATOM | 286 | N | ASP | A | 36 | 62.180 | 1.086 | 129.190 | 1.00 | 36.28 |
| ATOM | 287 | CA | ASP | A | 36 | 62.710 | 0.233 | 130.242 | 1.00 | 37.93 |
| ATOM | 288 | CB | ASP | A | 36 | 62.145 | -1.178 | 130.126 | 1.00 | 41.27 |
| ATOM | 289 | CG | ASP | A | 36 | 62.731 | -2.117 | 131.157 | 1.00 | 43.77 |
| ATOM | 290 | OD1 | ASP | A | 36 | 62.660 | -1.793 | 132.360 | 1.00 | 43.92 |
| ATOM | 291 | OD2 | ASP | A | 36 | 63.261 | -3.178 | 130.765 | 1.00 | 45.78 |
| ATOM | 292 | C | ASP | A | 36 | 64.227 | 0.181 | 130.174 | 1.00 | 38.74 |
| ATOM | 293 | O | ASP | A | 36 | 64.902 | 0.187 | 131.201 | 1.00 | 36.23 |
| ATOM | 294 | N | ALA | A | 37 | 64.760 | 0.127 | 128.958 | 1.00 | 37.96 |
| ATOM | 295 | CA | ALA | A | 37 | 66.201 | 0.080 | 128.768 | 1.00 | 39.49 |
| ATOM | 296 | CB | ALA | A | 37 | 66.525 | -0.158 | 127.299 | 1.00 | 39.74 |
| ATOM | 297 | C | ALA | A | 37 | 66.832 | 1.386 | 129.244 | 1.00 | 40.09 |
| ATOM | 298 | O | ALA | A | 37 | 67.962 | 1.402 | 129.714 | 1.00 | 38.80 |
| ATOM | 299 | N | MET | A | 38 | 66.085 | 2.477 | 129.131 | 1.00 | 39.04 |
| ATOM | 300 | CA | MET | A | 38 | 66.567 | 3.789 | 129.545 | 1.00 | 38.71 |
| ATOM | 301 | CB | MET | A | 38 | 65.965 | 4.863 | 128.640 | 1.00 | 36.66 |
| ATOM | 302 | CG | MET | A | 38 | 66.335 | 4.744 | 127.173 | 1.00 | 39.16 |
| ATOM | 303 | SD | MET | A | 38 | 68.005 | 5.298 | 126.840 | 1.00 | 37.55 |
| ATOM | 304 | CE | MET | A | 38 | 67.892 | 7.033 | 127.287 | 1.00 | 35.74 |
| ATOM | 305 | C | MET | A | 38 | 66.187 | 4.094 | 130.995 | 1.00 | 40.58 |
| ATOM | 306 | O | MET | A | 38 | 66.484 | 5.173 | 131.502 | 1.00 | 38.12 |
| ATOM | 307 | N | ASN | A | 39 | 65.530 | 3.147 | 131.657 | 1.00 | 38.41 |
| ATOM | 308 | CA | ASN | A | 39 | 65.094 | 3.346 | 133.039 | 1.00 | 42.46 |
| ATOM | 309 | CB | ASN | A | 39 | 66.298 | 3.494 | 133.979 | 1.00 | 46.06 |
| ATOM | 310 | CG | ASN | A | 39 | 67.125 | 2.224 | 134.074 | 1.00 | 51.69 |
| ATOM | 311 | OD1 | ASN | A | 39 | 66.625 | 2.175 | 134.487 | 1.00 | 54.33 |
| ATOM | 312 | ND2 | ASN | A | 39 | 68.396 | 2.313 | 133.695 | 1.00 | 49.13 |
| ATOM | 313 | C | ASN | A | 39 | 64.222 | 4.594 | 133.134 | 1.00 | 41.19 |
| ATOM | 314 | O | ASN | A | 39 | 64.375 | 5.402 | 134.050 | 1.00 | 42.74 |
| ATOM | 315 | N | LEU | A | 40 | 63.301 | 4.746 | 132.188 | 1.00 | 40.22 |
| ATOM | 316 | CA | LEU | A | 40 | 62.427 | 5.909 | 132.170 | 1.00 | 39.85 |
| ATOM | 317 | CB | LEU | A | 40 | 62.524 | 6.610 | 130.812 | 1.00 | 40.42 |
| ATOM | 318 | CG | LEU | A | 40 | 63.940 | 7.074 | 130.447 | 1.00 | 40.40 |
| ATOM | 319 | CD1 | LEU | A | 40 | 63.916 | 7.753 | 129.088 | 1.00 | 32.75 |
| ATOM | 320 | CD2 | LEU | A | 40 | 64.470 | 8.031 | 131.513 | 1.00 | 38.89 |
| ATOM | 321 | C | LEU | A | 40 | 60.967 | 5.610 | 132.505 | 1.00 | 38.97 |
| ATOM | 322 | O | LEU | A | 40 | 60.076 | 6.409 | 132.213 | 1.00 | 32.32 |
| ATOM | 323 | N | ILE | A | 41 | 60.720 | 4.461 | 133.124 | 1.00 | 38.57 |
| ATOM | 324 | CA | ILE | A | 41 | 59.363 | 4.109 | 133.520 | 1.00 | 42.43 |
| ATOM | 325 | CB | ILE | A | 41 | 58.536 | 3.575 | 132.330 | 1.00 | 39.13 |
| ATOM | 326 | CG2 | ILE | A | 41 | 59.137 | 2.271 | 131.820 | 1.00 | 36.51 |
| ATOM | 327 | CG1 | ILE | A | 41 | 57.082 | 3.367 | 132.774 | 1.00 | 38.71 |
| ATOM | 328 | CD1 | ILE | A | 41 | 56.147 | 2.920 | 131.676 | 1.00 | 44.09 |
| ATOM | 329 | C | ILE | A | 41 | 59.376 | 3.056 | 134.619 | 1.00 | 42.40 |
| ATOM | 330 | O | ILE | A | 41 | 60.255 | 2.195 | 134.654 | 1.00 | 43.05 |

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Figure 18-6

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|
| ATOM | 331 | N | ASP | A | 42 | 58.414 | 3.148 | 135.532 | 1.00 | 47.83 |
| ATOM | 332 | CA | ASP | A | 42 | 58.301 | 2.183 | 136.620 | 1.00 | 49.23 |
| ATOM | 333 | CB | ASP | A | 42 | 58.243 | 2.880 | 137.984 | 1.00 | 46.60 |
| ATOM | 334 | CG | ASP | A | 42 | 59.493 | 3.688 | 138.284 | 1.00 | 52.63 |
| ATOM | 335 | OD1 | ASP | A | 42 | 60.614 | 3.146 | 138.141 | 1.00 | 49.28 |
| ATOM | 336 | OD2 | ASP | A | 42 | 59.355 | 4.866 | 138.678 | 1.00 | 52.47 |
| ATOM | 337 | C | ASP | A | 42 | 57.034 | 1.368 | 136.405 | 1.00 | 51.22 |
| ATOM | 338 | O | ASP | A | 42 | 56.048 | 1.866 | 135.864 | 1.00 | 48.07 |
| ATOM | 339 | N | GLU | A | 43 | 57.072 | 0.111 | 136.832 | 1.00 | 51.41 |
| ATOM | 340 | CA | GLU | A | 43 | 55.945 | -0.792 | 136.673 | 1.00 | 50.67 |
| ATOM | 341 | CB | GLU | A | 43 | 56.234 | -2.094 | 137.412 | 1.00 | 54.49 |
| ATOM | 342 | CG | GLU | A | 43 | 55.208 | -3.178 | 137.185 | 1.00 | 60.55 |
| ATOM | 343 | CD | GLU | A | 43 | 55.524 | -4.432 | 137.974 | 1.00 | 66.12 |
| ATOM | 344 | OE1 | GLU | A | 43 | 54.761 | -5.417 | 137.861 | 1.00 | 70.33 |
| ATOM | 345 | OE2 | GLU | A | 43 | 56.536 | -4.427 | 138.711 | 1.00 | 67.39 |
| ATOM | 346 | C | GLU | A | 43 | 54.645 | -0.178 | 137.178 | 1.00 | 50.20 |
| ATOM | 347 | O | GLU | A | 43 | 53.567 | -0.475 | 136.658 | 1.00 | 48.27 |
| ATOM | 348 | N | LYS | A | 44 | 54.755 | 0.683 | 138.186 | 1.00 | 49.04 |
| ATOM | 349 | CA | LYS | A | 44 | 53.601 | 1.356 | 138.778 | 1.00 | 47.56 |
| ATOM | 350 | CB | LYS | A | 44 | 54.013 | 2.004 | 140.112 | 1.00 | 54.73 |
| ATOM | 351 | CG | LYS | A | 44 | 53.190 | 3.229 | 140.542 | 1.00 | 58.07 |
| ATOM | 352 | CD | LYS | A | 44 | 53.705 | 4.500 | 139.853 | 1.00 | 61.24 |
| ATOM | 353 | CE | LYS | A | 44 | 52.849 | 5.727 | 140.151 | 1.00 | 61.93 |
| ATOM | 354 | NZ | LYS | A | 44 | 51.501 | 5.644 | 139.519 | 1.00 | 62.80 |
| ATOM | 355 | C | LYS | A | 44 | 52.929 | 2.387 | 137.875 | 1.00 | 44.52 |
| ATOM | 356 | O | LYS | A | 44 | 51.752 | 2.701 | 138.052 | 1.00 | 45.31 |
| ATOM | 357 | N | GLU | A | 45 | 53.674 | 2.915 | 136.914 | 1.00 | 41.03 |
| ATOM | 358 | CA | GLU | A | 45 | 53.140 | 3.914 | 135.994 | 1.00 | 41.23 |
| ATOM | 359 | CB | GLU | A | 45 | 54.271 | 4.810 | 135.500 | 1.00 | 38.52 |
| ATOM | 360 | CG | GLU | A | 45 | 54.973 | 5.572 | 136.589 | 1.00 | 40.30 |
| ATOM | 361 | CD | GLU | A | 45 | 56.241 | 6.222 | 136.096 | 1.00 | 38.06 |
| ATOM | 362 | OE1 | GLU | A | 45 | 57.170 | 5.478 | 135.715 | 1.00 | 36.93 |
| ATOM | 363 | OE2 | GLU | A | 45 | 56.306 | 7.467 | 136.084 | 1.00 | 32.57 |
| ATOM | 364 | C | GLU | A | 45 | 52.479 | 3.253 | 134.791 | 1.00 | 40.69 |
| ATOM | 365 | O | GLU | A | 45 | 51.783 | 3.907 | 134.015 | 1.00 | 39.77 |
| ATOM | 366 | N | LEU | A | 46 | 52.700 | 1.953 | 134.645 | 1.00 | 36.90 |
| ATOM | 367 | CA | LEU | A | 46 | 52.165 | 1.207 | 133.517 | 1.00 | 40.46 |
| ATOM | 368 | CB | LEU | A | 46 | 53.222 | 0.219 | 133.034 | 1.00 | 35.52 |
| ATOM | 369 | CG | LEU | A | 46 | 52.873 | -0.619 | 131.811 | 1.00 | 43.75 |
| ATOM | 370 | CD1 | LEU | A | 46 | 52.571 | 0.292 | 130.630 | 1.00 | 42.06 |
| ATOM | 371 | CD2 | LEU | A | 46 | 54.035 | -1.544 | 131.500 | 1.00 | 42.90 |
| ATOM | 372 | C | LEU | A | 46 | 50.852 | 0.467 | 133.780 | 1.00 | 40.03 |
| ATOM | 373 | O | LEU | A | 46 | 50.741 | -0.306 | 134.730 | 1.00 | 39.37 |
| ATOM | 374 | N | ILE | A | 47 | 49.861 | 0.718 | 132.928 | 1.00 | 34.03 |
| ATOM | 375 | CA | ILE | A | 47 | 48.560 | 0.068 | 133.033 | 1.00 | 32.12 |
| ATOM | 376 | CB | ILE | A | 47 | 47.413 | 1.087 | 132.937 | 1.00 | 32.35 |
| ATOM | 377 | CG2 | ILE | A | 47 | 46.069 | 0.360 | 132.833 | 1.00 | 30.60 |
| ATOM | 378 | CG1 | ILE | A | 47 | 47.448 | 2.015 | 134.156 | 1.00 | 36.56 |
| ATOM | 379 | CD1 | ILE | A | 47 | 46.372 | 3.080 | 134.162 | 1.00 | 35.46 |
| ATOM | 380 | C | ILE | A | 47 | 48.428 | -0.920 | 131.882 | 1.00 | 33.67 |
| ATOM | 381 | O | ILE | A | 47 | 48.505 | -0.532 | 130.717 | 1.00 | 27.64 |
| ATOM | 382 | N | LYS | A | 48 | 48.231 | -2.195 | 132.205 | 1.00 | 32.98 |
| ATOM | 383 | CA | LYS | A | 48 | 48.102 | -3.224 | 131.176 | 1.00 | 30.98 |
| ATOM | 384 | CB | LYS | A | 48 | 48.038 | -4.609 | 131.821 | 1.00 | 39.21 |
| ATOM | 385 | CG | LYS | A | 48 | 47.956 | -5.747 | 130.819 | 1.00 | 46.81 |
| ATOM | 386 | CD | LYS | A | 48 | 47.989 | -7.102 | 131.509 | 1.00 | 50.75 |
| ATOM | 387 | CE | LYS | A | 48 | 47.967 | -8.240 | 130.492 | 1.00 | 54.43 |
| ATOM | 388 | NZ | LYS | A | 48 | 49.151 | -8.199 | 129.580 | 1.00 | 50.43 |
| ATOM | 389 | C | LYS | A | 48 | 46.869 | -3.006 | 130.310 | 1.00 | 29.55 |
| ATOM | 390 | C | LYS | A | 48 | 45.764 | -2.840 | 130.820 | 1.00 | 29.65 |
| ATOM | 391 | N | SER | A | 49 | 47.071 | -2.992 | 128.996 | 1.00 | 30.69 |
| ATOM | 392 | CA | SER | A | 49 | 45.989 | -2.802 | 128.033 | 1.00 | 29.32 |
| ATOM | 393 | CB | SER | A | 49 | 46.551 | -2.805 | 126.609 | 1.00 | 31.53 |
| ATOM | 394 | OG | SER | A | 49 | 47.571 | -1.834 | 126.443 | 1.00 | 30.74 |
| ATOM | 395 | C | SER | A | 49 | 44.952 | -3.916 | 128.147 | 1.00 | 31.31 |
| ATOM | 396 | O | SER | A | 49 | 45.295 | -5.059 | 128.436 | 1.00 | 34.44 |

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Figure 18-7

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|
| ATOM | 397 | N | ARG | A | 50 | 43.688 | -3.582 | 127.922 | 1.00 | 32.87 |
| ATOM | 398 | CA | ARG | A | 50 | 42.632 | -4.582 | 127.960 | 1.00 | 31.45 |
| ATOM | 399 | CB | ARG | A | 50 | 41.636 | -4.325 | 129.101 | 1.00 | 28.35 |
| ATOM | 400 | CG | ARG | A | 50 | 40.729 | -3.103 | 128.915 | 1.00 | 32.05 |
| ATOM | 401 | CD | ARG | A | 50 | 39.653 | -3.055 | 130.008 | 1.00 | 30.46 |
| ATOM | 402 | NE | ARG | A | 50 | 38.821 | -1.850 | 129.964 | 1.00 | 25.21 |
| ATOM | 403 | CZ | ARG | A | 50 | 37.930 | -1.569 | 129.016 | 1.00 | 28.32 |
| ATOM | 404 | NH1 | ARG | A | 50 | 37.726 | -2.406 | 128.001 | 1.00 | 25.45 |
| ATOM | 405 | NH2 | ARG | A | 50 | 37.238 | -0.439 | 129.087 | 1.00 | 24.92 |
| ATOM | 406 | C | ARG | A | 50 | 41.894 | -4.470 | 126.638 | 1.00 | 31.12 |
| ATOM | 407 | O | ARG | A | 50 | 41.895 | -3.406 | 126.019 | 1.00 | 24.62 |
| ATOM | 408 | N | PRO | A | 51 | 41.264 | -5.566 | 126.181 | 1.00 | 32.55 |
| ATOM | 409 | CD | PRO | A | 51 | 41.164 | -6.921 | 126.751 | 1.00 | 32.40 |
| ATOM | 410 | CA | PRO | A | 51 | 40.534 | -5.506 | 124.917 | 1.00 | 30.36 |
| ATOM | 411 | CB | PRO | A | 51 | 40.138 | -6.967 | 124.683 | 1.00 | 33.95 |
| ATOM | 412 | CG | PRO | A | 51 | 41.173 | -7.750 | 125.499 | 1.00 | 32.85 |
| ATOM | 413 | C | PRO | A | 51 | 39.309 | -4.630 | 125.134 | 1.00 | 31.61 |
| ATOM | 414 | O | PRO | A | 51 | 38.877 | -4.431 | 126.267 | 1.00 | 29.84 |
| ATOM | 415 | N | ALA | A | 52 | 38.755 | -4.093 | 124.058 | 1.00 | 29.09 |
| ATOM | 416 | CA | ALA | A | 52 | 37.556 | -3.294 | 124.183 | 1.00 | 29.61 |
| ATOM | 417 | CB | ALA | A | 52 | 37.365 | -2.447 | 122.956 | 1.00 | 28.67 |
| ATOM | 418 | C | ALA | A | 52 | 36.437 | -4.321 | 124.288 | 1.00 | 32.39 |
| ATOM | 419 | O | ALA | A | 52 | 36.603 | -5.453 | 123.844 | 1.00 | 30.40 |
| ATOM | 420 | N | THR | A | 53 | 35.318 | -3.947 | 124.896 | 1.00 | 32.98 |
| ATOM | 421 | CA | THR | A | 53 | 34.192 | -4.868 | 124.997 | 1.00 | 36.61 |
| ATOM | 422 | CB | THR | A | 53 | 33.253 | -4.514 | 126.166 | 1.00 | 34.22 |
| ATOM | 423 | OG1 | THR | A | 53 | 32.734 | -3.193 | 125.970 | 1.00 | 29.52 |
| ATOM | 424 | CG2 | THR | A | 53 | 33.998 | -4.579 | 127.493 | 1.00 | 36.45 |
| ATOM | 425 | C | THR | A | 53 | 33.411 | -4.700 | 123.702 | 1.00 | 38.94 |
| ATOM | 426 | O | THR | A | 53 | 33.559 | -3.689 | 123.012 | 1.00 | 32.67 |
| ATOM | 427 | N | LYS | A | 54 | 32.577 | -5.679 | 123.372 | 1.00 | 39.19 |
| ATOM | 428 | CA | LYS | A | 54 | 31.792 | -5.595 | 122.152 | 1.00 | 40.71 |
| ATOM | 429 | CB | LYS | A | 54 | 30.933 | -6.851 | 121.994 | 1.00 | 41.68 |
| ATOM | 430 | CG | LYS | A | 54 | 30.367 | -7.034 | 120.597 | 1.00 | 49.42 |
| ATOM | 431 | CD | LYS | A | 54 | 29.541 | -8.310 | 120.508 | 1.00 | 51.82 |
| ATOM | 432 | CE | LYS | A | 54 | 29.075 | -8.588 | 119.087 | 1.00 | 52.94 |
| ATOM | 433 | NZ | LYS | A | 54 | 30.216 | -8.879 | 118.182 | 1.00 | 54.26 |
| ATOM | 434 | C | LYS | A | 54 | 30.913 | -4.347 | 122.237 | 1.00 | 39.46 |
| ATOM | 435 | O | LYS | A | 54 | 30.719 | -3.637 | 121.249 | 1.00 | 37.19 |
| ATOM | 436 | N | GLU | A | 55 | 30.404 | -4.075 | 123.434 | 1.00 | 36.71 |
| ATOM | 437 | CA | GLU | A | 55 | 29.554 | -2.913 | 123.665 | 1.00 | 36.18 |
| ATOM | 438 | CB | GLU | A | 55 | 29.109 | -2.877 | 125.127 | 1.00 | 42.16 |
| ATOM | 439 | CG | GLU | A | 55 | 28.223 | -1.694 | 125.476 | 1.00 | 46.04 |
| ATOM | 440 | CD | GLU | A | 55 | 27.873 | -1.639 | 126.953 | 1.00 | 51.15 |
| ATOM | 441 | OE1 | GLU | A | 55 | 27.092 | -0.748 | 127.343 | 1.00 | 56.53 |
| ATOM | 442 | OE2 | GLU | A | 55 | 28.382 | -2.482 | 127.727 | 1.00 | 51.67 |
| ATOM | 443 | C | GLU | A | 55 | 30.278 | -1.607 | 123.327 | 1.00 | 35.45 |
| ATOM | 444 | O | GLU | A | 55 | 29.721 | -0.729 | 122.667 | 1.00 | 29.11 |
| ATOM | 445 | N | GLU | A | 56 | 31.518 | -1.476 | 123.776 | 1.00 | 27.82 |
| ATOM | 446 | CA | GLU | A | 56 | 32.289 | -0.269 | 123.497 | 1.00 | 34.70 |
| ATOM | 447 | CB | GLU | A | 56 | 33.635 | -0.329 | 124.232 | 1.00 | 30.71 |
| ATOM | 448 | CG | GLU | A | 56 | 33.474 | -0.484 | 125.746 | 1.00 | 35.09 |
| ATOM | 449 | CD | GLU | A | 56 | 34.787 | -0.675 | 126.479 | 1.00 | 32.29 |
| ATOM | 450 | OE1 | GLU | A | 56 | 35.645 | -1.434 | 125.986 | 1.00 | 34.54 |
| ATOM | 451 | OE2 | GLU | A | 56 | 34.951 | -0.094 | 127.569 | 1.00 | 33.25 |
| ATOM | 452 | C | GLU | A | 56 | 32.495 | -0.104 | 121.988 | 1.00 | 32.51 |
| ATOM | 453 | O | GLU | A | 56 | 32.341 | 0.990 | 121.444 | 1.00 | 29.59 |
| ATOM | 454 | N | LEU | A | 57 | 32.827 | -1.196 | 121.311 | 1.00 | 35.58 |
| ATOM | 455 | CA | LEU | A | 57 | 33.039 | -1.147 | 119.871 | 1.00 | 35.70 |
| ATOM | 456 | CB | LEU | A | 57 | 33.475 | -2.512 | 119.334 | 1.00 | 35.25 |
| ATOM | 457 | CG | LEU | A | 57 | 34.829 | -3.030 | 119.814 | 1.00 | 36.19 |
| ATOM | 458 | CD1 | LEU | A | 57 | 35.095 | -4.390 | 119.183 | 1.00 | 33.69 |
| ATOM | 459 | CD2 | LEU | A | 57 | 35.925 | -2.041 | 119.433 | 1.00 | 32.61 |
| ATOM | 460 | C | LEU | A | 57 | 31.772 | -0.717 | 119.157 | 1.00 | 36.02 |
| ATOM | 461 | O | LEU | A | 57 | 31.828 | 0.067 | 118.205 | 1.00 | 32.72 |
| ATOM | 462 | N | LEU | A | 58 | 30.631 | -1.228 | 119.620 | 1.00 | 32.35 |

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Figure 18-8

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|
| ATOM | 463 | CA | LEU | A | 58 | 29.353 | -0.898 | 119.004 | 1.00 | 33.21 |
| ATOM | 464 | CB | LEU | A | 58 | 28.260 | -1.844 | 119.495 | 1.00 | 35.17 |
| ATOM | 465 | CG | LEU | A | 58 | 28.504 | -3.296 | 119.077 | 1.00 | 33.71 |
| ATOM | 466 | CD1 | LEU | A | 58 | 27.338 | -4.166 | 119.524 | 1.00 | 36.80 |
| ATOM | 467 | CD2 | LEU | A | 58 | 28.665 | -3.364 | 117.570 | 1.00 | 36.50 |
| ATOM | 468 | C | LEU | A | 58 | 28.940 | -0.543 | 119.222 | 1.00 | 30.99 |
| ATOM | 469 | O | LEU | A | 58 | 27.915 | 0.985 | 118.700 | 1.00 | 35.50 |
| ATOM | 470 | N | LEU | A | 59 | 29.733 | 1.279 | 119.993 | 1.00 | 32.55 |
| ATOM | 471 | CA | LEU | A | 59 | 29.443 | 2.687 | 120.217 | 1.00 | 30.37 |
| ATOM | 472 | CB | LEU | A | 59 | 30.387 | 3.279 | 121.268 | 1.00 | 28.01 |
| ATOM | 473 | CG | LEU | A | 59 | 30.174 | 2.828 | 122.716 | 1.00 | 32.19 |
| ATOM | 474 | CD1 | LEU | A | 59 | 31.248 | 3.427 | 123.604 | 1.00 | 24.85 |
| ATOM | 475 | CD2 | LEU | A | 59 | 28.785 | 3.263 | 123.192 | 1.00 | 25.65 |
| ATOM | 476 | C | LEU | A | 59 | 29.632 | 3.405 | 118.890 | 1.00 | 31.26 |
| ATOM | 477 | O | LEU | A | 59 | 29.020 | 4.442 | 118.652 | 1.00 | 31.80 |
| ATOM | 478 | N | PHE | A | 60 | 30.482 | 2.850 | 118.026 | 1.00 | 29.79 |
| ATOM | 479 | CA | PHE | A | 60 | 30.726 | 3.454 | 116.716 | 1.00 | 30.24 |
| ATOM | 480 | CB | PHE | A | 60 | 32.131 | 4.055 | 116.637 | 1.00 | 29.99 |
| ATOM | 481 | CG | PHE | A | 60 | 32.443 | 4.691 | 115.299 | 1.00 | 28.88 |
| ATOM | 482 | CD1 | PHE | A | 60 | 31.706 | 5.780 | 114.845 | 1.00 | 25.58 |
| ATOM | 483 | CD2 | PHE | A | 60 | 33.448 | 4.178 | 114.479 | 1.00 | 24.00 |
| ATOM | 484 | CE1 | PHE | A | 60 | 31.959 | 6.351 | 113.592 | 1.00 | 26.12 |
| ATOM | 485 | CE2 | PHE | A | 60 | 33.709 | 4.740 | 113.226 | 1.00 | 25.98 |
| ATOM | 486 | CZ | PHE | A | 60 | 32.963 | 5.828 | 112.781 | 1.00 | 24.53 |
| ATOM | 487 | C | PHE | A | 60 | 30.536 | 2.520 | 115.529 | 1.00 | 30.30 |
| ATOM | 488 | O | PHE | A | 60 | 29.810 | 2.854 | 114.602 | 1.00 | 32.82 |
| ATOM | 489 | N | HIS | A | 61 | 31.195 | 1.363 | 115.543 | 1.00 | 32.85 |
| ATOM | 490 | CA | HIS | A | 61 | 31.075 | 0.418 | 114.431 | 1.00 | 34.59 |
| ATOM | 491 | CB | HIS | A | 61 | 32.296 | -0.492 | 114.361 | 1.00 | 32.89 |
| ATOM | 492 | CG | HIS | A | 61 | 33.576 | 0.238 | 114.116 | 1.00 | 34.25 |
| ATOM | 493 | CD2 | HIS | A | 61 | 34.225 | 0.532 | 112.967 | 1.00 | 34.67 |
| ATOM | 494 | ND1 | HIS | A | 61 | 34.328 | 0.786 | 115.133 | 1.00 | 37.78 |
| ATOM | 495 | CE1 | HIS | A | 61 | 35.390 | 1.382 | 114.619 | 1.00 | 37.50 |
| ATOM | 496 | NE2 | HIS | A | 61 | 35.350 | 1.243 | 113.307 | 1.00 | 37.91 |
| ATOM | 497 | C | HIS | A | 61 | 29.824 | -0.449 | 114.480 | 1.00 | 38.44 |
| ATOM | 498 | O | HIS | A | 61 | 29.213 | -0.612 | 115.538 | 1.00 | 35.78 |
| ATOM | 499 | N | THR | A | 62 | 29.462 | -1.015 | 113.327 | 1.00 | 39.73 |
| ATOM | 500 | CA | THR | A | 62 | 28.278 | -1.868 | 113.218 | 1.00 | 38.05 |
| ATOM | 501 | CB | THR | A | 62 | 27.682 | -1.825 | 111.804 | 1.00 | 37.22 |
| ATOM | 502 | OG1 | THR | A | 62 | 28.631 | -2.345 | 110.867 | 1.00 | 41.15 |
| ATOM | 503 | CG2 | THR | A | 62 | 27.348 | -0.404 | 111.418 | 1.00 | 38.27 |
| ATOM | 504 | C | THR | A | 62 | 28.598 | -3.317 | 113.551 | 1.00 | 39.06 |
| ATOM | 505 | O | THR | A | 62 | 29.731 | -3.768 | 113.392 | 1.00 | 39.32 |
| ATOM | 506 | N | GLU | A | 63 | 27.582 | -4.034 | 114.017 | 1.00 | 40.92 |
| ATOM | 507 | CA | GLU | A | 63 | 27.696 | -5.441 | 114.393 | 1.00 | 40.68 |
| ATOM | 508 | CB | GLU | A | 63 | 26.303 | -6.000 | 114.704 | 1.00 | 43.19 |
| ATOM | 509 | CG | GLU | A | 63 | 26.269 | -7.451 | 115.171 | 1.00 | 46.90 |
| ATOM | 510 | CD | GLU | A | 63 | 26.472 | -7.593 | 116.665 | 1.00 | 53.11 |
| ATOM | 511 | OE1 | GLU | A | 63 | 26.601 | -8.739 | 117.152 | 1.00 | 52.78 |
| ATOM | 512 | OE2 | GLU | A | 63 | 26.487 | -6.556 | 117.358 | 1.00 | 57.24 |
| ATOM | 513 | C | GLU | A | 63 | 28.320 | -6.263 | 113.268 | 1.00 | 36.19 |
| ATOM | 514 | O | GLU | A | 63 | 29.272 | -7.011 | 113.481 | 1.00 | 29.70 |
| ATOM | 515 | N | ASP | A | 64 | 27.755 | -6.119 | 112.074 | 1.00 | 35.85 |
| ATOM | 516 | CA | ASP | A | 64 | 28.198 | -6.841 | 110.886 | 1.00 | 37.61 |
| ATOM | 517 | CB | ASP | A | 64 | 27.363 | -6.382 | 109.697 | 1.00 | 43.30 |
| ATOM | 518 | CG | ASP | A | 64 | 27.313 | -4.872 | 109.582 | 1.00 | 53.38 |
| ATOM | 519 | OD1 | ASP | A | 64 | 28.290 | -4.269 | 109.089 | 1.00 | 52.15 |
| ATOM | 520 | OD2 | ASP | A | 64 | 26.298 | -4.285 | 110.018 | 1.00 | 53.97 |
| ATOM | 521 | C | ASP | A | 64 | 29.673 | -6.660 | 110.594 | 1.00 | 35.04 |
| ATOM | 522 | O | ASP | A | 64 | 30.379 | -7.625 | 110.303 | 1.00 | 33.60 |
| ATOM | 523 | N | TYR | A | 65 | 30.144 | -5.423 | 110.671 | 1.00 | 33.88 |
| ATOM | 524 | CA | TYR | A | 65 | 31.554 | -5.153 | 110.419 | 1.00 | 32.91 |
| ATOM | 525 | CB | TYR | A | 65 | 31.793 | -3.637 | 110.375 | 1.00 | 34.80 |
| ATOM | 526 | CG | TYR | A | 65 | 33.247 | -3.253 | 110.219 | 1.00 | 35.19 |
| ATOM | 527 | CD1 | TYR | A | 65 | 34.009 | -3.751 | 109.163 | 1.00 | 28.43 |
| ATOM | 528 | CE1 | TYR | A | 65 | 35.352 | -3.411 | 109.024 | 1.00 | 32.52 |

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Figure 18-9

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|---------|------|-------|
| ATOM | 529 | CD2 | TYR | A | 65 | 33.863 | -2.398 | 111.134 | 1.00 | 34.08 |
| ATOM | 530 | CE2 | TYR | A | 65 | 35.211 | -2.050 | 111.002 | 1.00 | 29.89 |
| ATOM | 531 | CZ | TYR | A | 65 | 35.949 | -2.560 | 109.948 | 1.00 | 35.29 |
| ATOM | 532 | OH | TYR | A | 65 | 37.286 | -2.231 | 109.825 | 1.00 | 29.81 |
| ATOM | 533 | C | TYR | A | 65 | 32.405 | -5.813 | 111.504 | 1.00 | 27.65 |
| ATOM | 534 | O | TYR | A | 65 | 33.339 | -6.557 | 111.209 | 1.00 | 27.65 |
| ATOM | 535 | N | ILE | A | 66 | 32.070 | -5.559 | 112.765 | 1.00 | 27.32 |
| ATOM | 536 | CA | ILE | A | 66 | 32.822 | -6.153 | 113.858 | 1.00 | 25.82 |
| ATOM | 537 | CB | ILE | A | 66 | 32.227 | -5.764 | 115.217 | 1.00 | 32.25 |
| ATOM | 538 | CG2 | ILE | A | 66 | 33.029 | -6.403 | 116.338 | 1.00 | 28.85 |
| ATOM | 539 | CG1 | ILE | A | 66 | 32.226 | -4.242 | 115.364 | 1.00 | 31.48 |
| ATOM | 540 | CD1 | ILE | A | 66 | 33.607 | -3.612 | 115.282 | 1.00 | 38.02 |
| ATOM | 541 | C | ILE | A | 66 | 32.836 | -7.677 | 113.736 | 1.00 | 31.21 |
| ATOM | 542 | O | ILE | A | 66 | 33.891 | -8.305 | 113.844 | 1.00 | 30.25 |
| ATOM | 543 | N | ASN | A | 67 | 31.672 | -8.279 | 113.507 | 1.00 | 33.28 |
| ATOM | 544 | CA | ASN | A | 67 | 31.627 | -9.731 | 113.372 | 1.00 | 35.87 |
| ATOM | 545 | CB | ASN | A | 67 | 30.190 | -10.242 | 113.177 | 1.00 | 33.07 |
| ATOM | 546 | CG | ASN | A | 67 | 29.338 | -10.072 | 114.421 | 1.00 | 37.34 |
| ATOM | 547 | OD1 | ASN | A | 67 | 29.807 | -10.296 | 115.535 | 1.00 | 35.20 |
| ATOM | 548 | ND2 | ASN | A | 67 | 28.071 | -9.709 | 114.236 | 1.00 | 34.83 |
| ATOM | 549 | C | ASN | A | 67 | 32.499 | -10.198 | 112.219 | 1.00 | 31.00 |
| ATOM | 550 | O | ASN | A | 67 | 33.132 | -11.248 | 112.306 | 1.00 | 37.26 |
| ATOM | 551 | N | THR | A | 68 | 32.543 | -9.426 | 111.140 | 1.00 | 30.91 |
| ATOM | 552 | CA | THR | A | 68 | 33.368 | -9.814 | 109.997 | 1.00 | 31.04 |
| ATOM | 553 | CB | THR | A | 68 | 33.133 | -8.894 | 108.792 | 1.00 | 34.01 |
| ATOM | 554 | OG1 | THR | A | 68 | 31.780 | -9.037 | 108.352 | 1.00 | 33.26 |
| ATOM | 555 | CG2 | THR | A | 68 | 34.072 | -9.256 | 107.646 | 1.00 | 30.84 |
| ATOM | 556 | C | THR | A | 68 | 34.844 | -9.794 | 110.378 | 1.00 | 33.31 |
| ATOM | 557 | O | THR | A | 68 | 35.591 | -10.708 | 110.024 | 1.00 | 32.52 |
| ATOM | 558 | N | LEU | A | 69 | 35.267 | -8.768 | 111.117 | 1.00 | 30.30 |
| ATOM | 559 | CA | LEU | A | 69 | 36.669 | -8.686 | 111.534 | 1.00 | 28.20 |
| ATOM | 560 | CB | LEU | A | 69 | 36.938 | -7.409 | 112.351 | 1.00 | 28.25 |
| ATOM | 561 | CG | LEU | A | 69 | 36.859 | -6.049 | 111.647 | 1.00 | 30.18 |
| ATOM | 562 | CD1 | LEU | A | 69 | 37.154 | -4.929 | 112.647 | 1.00 | 31.08 |
| ATOM | 563 | CD2 | LEU | A | 69 | 37.868 | -6.004 | 110.505 | 1.00 | 27.85 |
| ATOM | 564 | C | LEU | A | 69 | 37.036 | -9.902 | 112.372 | 1.00 | 31.65 |
| ATOM | 565 | O | LEU | A | 69 | 38.084 | -10.519 | 112.165 | 1.00 | 23.95 |
| ATOM | 566 | N | MET | A | 70 | 36.169 | -10.243 | 113.321 | 1.00 | 30.78 |
| ATOM | 567 | CA | MET | A | 70 | 36.411 | -11.383 | 114.193 | 1.00 | 34.50 |
| ATOM | 568 | CB | MET | A | 70 | 35.318 | -11.486 | 115.258 | 1.00 | 31.96 |
| ATOM | 569 | CG | MET | A | 70 | 35.203 | -10.259 | 116.147 | 1.00 | 36.26 |
| ATOM | 570 | SD | MET | A | 70 | 33.948 | -10.454 | 117.431 | 1.00 | 37.52 |
| ATOM | 571 | CE | MET | A | 70 | 34.633 | -11.815 | 118.403 | 1.00 | 37.36 |
| ATOM | 572 | C | MET | A | 70 | 36.484 | -12.685 | 113.401 | 1.00 | 33.33 |
| ATOM | 573 | O | MET | A | 70 | 37.392 | -13.488 | 113.607 | 1.00 | 31.47 |
| ATOM | 574 | N | GLU | A | 71 | 35.534 | -12.887 | 112.494 | 1.00 | 35.37 |
| ATOM | 575 | CA | GLU | A | 71 | 35.516 | -14.098 | 111.681 | 1.00 | 36.6 |
| ATOM | 576 | CB | GLU | A | 71 | 34.245 | -14.160 | 110.834 | 1.00 | 37.3 |
| ATOM | 577 | CG | GLU | A | 71 | 34.206 | -15.359 | 109.897 | 1.00 | 46.37 |
| ATOM | 578 | CD | GLU | A | 71 | 34.257 | -16.693 | 110.633 | 1.00 | 46.37 |
| ATOM | 579 | OE1 | GLU | A | 71 | 34.355 | -17.733 | 109.952 | 1.00 | 48.94 |
| ATOM | 580 | OE2 | GLU | A | 71 | 34.190 | -16.705 | 111.882 | 1.00 | 45.53 |
| ATOM | 581 | C | GLU | A | 71 | 36.732 | -14.169 | 110.769 | 1.00 | 35.96 |
| ATOM | 582 | O | GLU | A | 71 | 37.342 | -15.228 | 110.617 | 1.00 | 32.99 |
| ATOM | 583 | N | ALA | A | 72 | 37.079 | -13.039 | 110.159 | 1.00 | 36.50 |
| ATOM | 584 | CA | ALA | A | 72 | 38.225 | -12.981 | 109.264 | 1.00 | 33.98 |
| ATOM | 585 | CB | ALA | A | 72 | 38.366 | -11.580 | 108.675 | 1.00 | 33.23 |
| ATOM | 586 | C | ALA | A | 72 | 39.498 | -13.362 | 109.998 | 1.00 | 34.60 |
| ATOM | 587 | O | ALA | A | 72 | 40.337 | -14.094 | 109.466 | 1.00 | 31.53 |
| ATOM | 588 | N | GLU | A | 73 | 39.647 | -12.873 | 111.224 | 1.00 | 30.87 |
| ATOM | 589 | CA | GLU | A | 73 | 40.847 | -13.177 | 111.985 | 1.00 | 29.66 |
| ATOM | 590 | CB | GLU | A | 73 | 41.004 | -12.224 | 113.180 | 1.00 | 33.33 |
| ATOM | 591 | CG | GLU | A | 73 | 42.234 | -12.545 | 114.033 | 1.00 | 32.80 |
| ATOM | 592 | CD | GLU | A | 73 | 42.390 | -11.634 | 115.233 | 1.00 | 40.07 |
| ATOM | 593 | OE1 | GLU | A | 73 | 42.601 | -10.418 | 115.044 | 1.00 | 41.02 |
| ATOM | 594 | OE2 | GLU | A | 73 | 42.298 | -12.138 | 116.372 | 1.00 | 41.21 |

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Figure 18-10

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|---------|------|-------|
| ATOM | 595 | C | GLU | A | 73 | 40.906 | -14.615 | 112.485 | 1.00 | 31.73 |
| ATOM | 596 | O | GLU | A | 73 | 41.957 | -15.249 | 112.409 | 1.00 | 32.96 |
| ATOM | 597 | N | ARG | A | 74 | 39.798 | -15.145 | 112.992 | 1.00 | 35.85 |
| ATOM | 598 | CA | ARG | A | 74 | 39.847 | -16.511 | 113.502 | 1.00 | 43.24 |
| ATOM | 599 | CB | ARG | A | 74 | 38.548 | -16.892 | 114.216 | 1.00 | 43.63 |
| ATOM | 600 | CG | ARG | A | 74 | 37.450 | -17.349 | 113.294 | 1.00 | 51.20 |
| ATOM | 601 | CD | ARG | A | 74 | 36.366 | -18.087 | 114.063 | 1.00 | 51.13 |
| ATOM | 602 | NE | ARG | A | 74 | 35.534 | -18.871 | 113.158 | 1.00 | 57.40 |
| ATOM | 603 | CZ | ARG | A | 74 | 35.991 | -19.870 | 112.403 | 1.00 | 56.36 |
| ATOM | 604 | NH1 | ARG | A | 74 | 37.273 | -20.208 | 112.446 | 1.00 | 51.10 |
| ATOM | 605 | NH2 | ARG | A | 74 | 35.172 | -20.517 | 111.586 | 1.00 | 58.75 |
| ATOM | 606 | C | ARG | A | 74 | 40.125 | -17.506 | 112.372 | 1.00 | 43.06 |
| ATOM | 607 | O | ARG | A | 74 | 40.916 | -18.429 | 112.541 | 1.00 | 42.52 |
| ATOM | 608 | N | SER | A | 75 | 39.485 | -17.305 | 111.222 | 1.00 | 43.63 |
| ATOM | 609 | CA | SER | A | 75 | 39.670 | -18.186 | 110.066 | 1.00 | 44.93 |
| ATOM | 610 | CB | SER | A | 75 | 38.485 | -18.089 | 109.113 | 1.00 | 42.05 |
| ATOM | 611 | OG | SER | A | 75 | 38.420 | -16.799 | 108.532 | 1.00 | 38.43 |
| ATOM | 612 | C | SER | A | 75 | 40.910 | -17.797 | 109.282 | 1.00 | 46.44 |
| ATOM | 613 | O | SER | A | 75 | 41.339 | -18.522 | 108.383 | 1.00 | 45.17 |
| ATOM | 614 | N | GLN | A | 76 | 41.466 | -16.638 | 109.618 | 1.00 | 46.18 |
| ATOM | 615 | CA | GLN | A | 76 | 42.642 | -16.116 | 108.936 | 1.00 | 44.73 |
| ATOM | 616 | CB | GLN | A | 76 | 43.868 | -16.973 | 109.226 | 1.00 | 37.36 |
| ATOM | 617 | CG | GLN | A | 76 | 45.162 | -16.208 | 109.045 | 1.00 | 43.96 |
| ATOM | 618 | CD | GLN | A | 76 | 45.415 | -15.214 | 110.176 | 1.00 | 41.86 |
| ATOM | 619 | OE1 | GLN | A | 76 | 44.499 | -14.537 | 110.655 | 1.00 | 37.78 |
| ATOM | 620 | NE2 | GLN | A | 76 | 46.669 | -15.111 | 110.591 | 1.00 | 45.00 |
| ATOM | 621 | C | GLN | A | 76 | 42.374 | -16.120 | 107.429 | 1.00 | 44.17 |
| ATOM | 622 | O | GLN | A | 76 | 43.233 | -16.495 | 106.630 | 1.00 | 40.49 |
| ATOM | 623 | N | SER | A | 77 | 41.168 | -15.713 | 107.053 | 1.00 | 43.11 |
| ATOM | 624 | CA | SER | A | 77 | 40.784 | -15.667 | 105.649 | 1.00 | 44.66 |
| ATOM | 625 | CB | SER | A | 77 | 40.182 | -17.004 | 105.220 | 1.00 | 44.56 |
| ATOM | 626 | OG | SER | A | 77 | 38.974 | -17.246 | 105.925 | 1.00 | 42.58 |
| ATOM | 627 | C | SER | A | 77 | 39.747 | -14.573 | 105.448 | 1.00 | 44.80 |
| ATOM | 628 | O | SER | A | 77 | 39.096 | -14.142 | 106.395 | 1.00 | 45.11 |
| ATOM | 629 | N | VAL | A | 78 | 39.590 | -14.137 | 104.207 | 1.00 | 46.06 |
| ATOM | 630 | CA | VAL | A | 78 | 38.632 | -13.095 | 103.888 | 1.00 | 47.65 |
| ATOM | 631 | CB | VAL | A | 78 | 39.107 | -12.245 | 102.701 | 1.00 | 49.63 |
| ATOM | 632 | CG1 | VAL | A | 78 | 38.076 | -11.167 | 102.391 | 1.00 | 51.25 |
| ATOM | 633 | CG2 | VAL | A | 78 | 40.454 | -11.627 | 103.017 | 1.00 | 53.00 |
| ATOM | 634 | C | VAL | A | 78 | 37.275 | -13.682 | 103.530 | 1.00 | 48.07 |
| ATOM | 635 | O | VAL | A | 78 | 37.111 | -14.301 | 102.480 | 1.00 | 42.31 |
| ATOM | 636 | N | PRO | A | 79 | 36.282 | -13.492 | 104.407 | 1.00 | 49.82 |
| ATOM | 637 | CD | PRO | A | 79 | 36.347 | -12.782 | 105.696 | 1.00 | 50.81 |
| ATOM | 638 | CA | PRO | A | 79 | 34.927 | -13.998 | 104.186 | 1.00 | 51.31 |
| ATOM | 639 | CB | PRO | A | 79 | 34.170 | -13.450 | 105.396 | 1.00 | 53.13 |
| ATOM | 640 | CG | PRO | A | 79 | 35.244 | -13.469 | 106.469 | 1.00 | 53.50 |
| ATOM | 641 | C | PRO | A | 79 | 34.343 | -13.517 | 102.858 | 1.00 | 52.42 |
| ATOM | 642 | O | PRO | A | 79 | 34.670 | -12.428 | 102.382 | 1.00 | 55.73 |
| ATOM | 643 | N | LYS | A | 80 | 33.482 | -14.343 | 102.273 | 1.00 | 49.63 |
| ATOM | 644 | CA | LYS | A | 80 | 32.824 | -14.053 | 101.002 | 1.00 | 51.62 |
| ATOM | 645 | CB | LYS | A | 80 | 31.632 | -15.004 | 100.822 | 1.00 | 53.92 |
| ATOM | 646 | CG | LYS | A | 80 | 30.817 | -14.808 | 99.545 | 1.00 | 56.27 |
| ATOM | 647 | CD | LYS | A | 80 | 29.586 | -15.712 | 99.560 | 1.00 | 56.61 |
| ATOM | 648 | CE | LYS | A | 80 | 28.744 | -15.579 | 98.298 | 1.00 | 56.04 |
| ATOM | 649 | NZ | LYS | A | 80 | 29.471 | -16.036 | 97.081 | 1.00 | 58.90 |
| ATOM | 650 | C | LYS | A | 80 | 32.338 | -12.607 | 100.874 | 1.00 | 51.10 |
| ATOM | 651 | O | LYS | A | 80 | 31.539 | -12.140 | 101.689 | 1.00 | 49.22 |
| ATOM | 652 | N | GLY | A | 81 | 32.821 | -11.914 | 99.842 | 1.00 | 51.14 |
| ATOM | 653 | CA | GLY | A | 81 | 32.418 | -10.537 | 99.592 | 1.00 | 47.07 |
| ATOM | 654 | C | GLY | A | 81 | 32.876 | -9.496 | 100.599 | 1.00 | 46.90 |
| ATOM | 655 | O | GLY | A | 81 | 32.671 | -8.301 | 100.397 | 1.00 | 43.90 |
| ATOM | 656 | N | ALA | A | 82 | 33.504 | -9.942 | 101.681 | 1.00 | 44.50 |
| ATOM | 657 | CA | ALA | A | 82 | 33.973 | -9.029 | 102.715 | 1.00 | 44.69 |
| ATOM | 658 | CB | ALA | A | 82 | 34.497 | -9.825 | 103.903 | 1.00 | 44.62 |
| ATOM | 659 | C | ALA | A | 82 | 35.049 | -8.073 | 102.215 | 1.00 | 41.82 |
| ATOM | 660 | O | ALA | A | 82 | 35.132 | -6.925 | 102.662 | 1.00 | 35.92 |

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Figure 18-11

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|
| ATOM | 661 | N | ARG | A | 83 | 35.874 | -8.549 | 101.289 | 1.00 | 43.30 |
| ATOM | 662 | CA | ARG | A | 83 | 36.959 | -7.742 | 100.741 | 1.00 | 43.25 |
| ATOM | 663 | CB | ARG | A | 83 | 37.715 | -8.533 | 99.677 | 1.00 | 46.60 |
| ATOM | 664 | CG | ARG | A | 83 | 38.988 | -7.865 | 99.222 | 1.00 | 51.32 |
| ATOM | 665 | CD | ARG | A | 83 | 39.636 | -8.632 | 98.086 | 1.00 | 55.55 |
| ATOM | 666 | NE | ARG | A | 83 | 40.995 | -8.164 | 97.810 | 1.00 | 64.08 |
| ATOM | 667 | CZ | ARG | A | 83 | 41.330 | -6.905 | 97.540 | 1.00 | 63.01 |
| ATOM | 668 | NH1 | ARG | A | 83 | 40.403 | -5.954 | 97.504 | 1.00 | 62.76 |
| ATOM | 669 | NH2 | ARG | A | 83 | 42.599 | -6.600 | 97.304 | 1.00 | 59.66 |
| ATOM | 670 | C | ARG | A | 83 | 36.453 | -6.435 | 100.134 | 1.00 | 44.58 |
| ATOM | 671 | O | ARG | A | 83 | 37.002 | -5.365 | 100.395 | 1.00 | 38.05 |
| ATOM | 672 | N | GLU | A | 84 | 35.404 | -6.528 | 99.323 | 1.00 | 41.82 |
| ATOM | 673 | CA | GLU | A | 84 | 34.824 | -5.356 | 98.678 | 1.00 | 41.44 |
| ATOM | 674 | CB | GLU | A | 84 | 34.145 | -5.765 | 97.367 | 1.00 | 46.27 |
| ATOM | 675 | CG | GLU | A | 84 | 33.621 | -7.185 | 97.388 | 1.00 | 52.61 |
| ATOM | 676 | CD | GLU | A | 84 | 34.749 | -8.198 | 97.308 | 1.00 | 54.12 |
| ATOM | 677 | OE1 | GLU | A | 84 | 34.555 | -9.344 | 97.764 | 1.00 | 59.66 |
| ATOM | 678 | OE2 | GLU | A | 84 | 35.823 | -7.850 | 96.769 | 1.00 | 50.30 |
| ATOM | 679 | C | GLU | A | 84 | 33.831 | -4.595 | 99.545 | 1.00 | 37.36 |
| ATOM | 680 | O | GLU | A | 84 | 33.692 | -3.379 | 99.416 | 1.00 | 34.30 |
| ATOM | 681 | N | LYS | A | 85 | 33.138 | -5.301 | 100.427 | 1.00 | 36.00 |
| ATOM | 682 | CA | LYS | A | 85 | 32.154 | -4.646 | 101.280 | 1.00 | 36.95 |
| ATOM | 683 | CB | LYS | A | 85 | 31.089 | -5.649 | 101.725 | 1.00 | 36.60 |
| ATOM | 684 | CG | LYS | A | 85 | 29.975 | -5.042 | 102.570 | 1.00 | 40.72 |
| ATOM | 685 | CD | LYS | A | 85 | 28.939 | -6.092 | 102.963 | 1.00 | 46.21 |
| ATOM | 686 | CE | LYS | A | 85 | 27.839 | -5.487 | 103.827 | 1.00 | 49.06 |
| ATOM | 687 | NZ | LYS | A | 85 | 26.859 | -6.513 | 104.287 | 1.00 | 52.72 |
| ATOM | 688 | C | LYS | A | 85 | 32.785 | -4.008 | 102.513 | 1.00 | 36.48 |
| ATOM | 689 | O | LYS | A | 85 | 32.353 | -2.949 | 102.966 | 1.00 | 32.97 |
| ATOM | 690 | N | TYR | A | 86 | 33.819 | -4.649 | 103.041 | 1.00 | 33.69 |
| ATOM | 691 | CA | TYR | A | 86 | 34.468 | -4.169 | 104.250 | 1.00 | 35.23 |
| ATOM | 692 | CB | TYR | A | 86 | 34.410 | -5.281 | 105.300 | 1.00 | 33.65 |
| ATOM | 693 | CG | TYR | A | 86 | 32.990 | -5.665 | 105.680 | 1.00 | 35.09 |
| ATOM | 694 | CD1 | TYR | A | 86 | 32.165 | -4.765 | 106.351 | 1.00 | 34.06 |
| ATOM | 695 | CE1 | TYR | A | 86 | 30.866 | -5.100 | 106.704 | 1.00 | 34.32 |
| ATOM | 696 | CD2 | TYR | A | 86 | 32.470 | -6.923 | 105.365 | 1.00 | 33.17 |
| ATOM | 697 | CE2 | TYR | A | 86 | 31.162 | -7.271 | 105.716 | 1.00 | 33.91 |
| ATOM | 698 | CZ | TYR | A | 86 | 30.369 | -6.350 | 106.386 | 1.00 | 34.21 |
| ATOM | 699 | OH | TYR | A | 86 | 29.079 | -6.658 | 106.738 | 1.00 | 35.20 |
| ATOM | 700 | C | TYR | A | 86 | 35.901 | -3.672 | 104.046 | 1.00 | 36.09 |
| ATOM | 701 | O | TYR | A | 86 | 36.552 | -3.208 | 104.984 | 1.00 | 36.06 |
| ATOM | 702 | N | ASN | A | 87 | 36.382 | -3.777 | 102.814 | 1.00 | 36.46 |
| ATOM | 703 | CA | ASN | A | 87 | 37.712 | -3.313 | 102.441 | 1.00 | 32.71 |
| ATOM | 704 | CB | ASN | A | 87 | 37.768 | -1.791 | 102.576 | 1.00 | 36.26 |
| ATOM | 705 | CG | ASN | A | 87 | 38.989 | -1.199 | 101.926 | 1.00 | 37.25 |
| ATOM | 706 | OD1 | ASN | A | 87 | 39.305 | -1.518 | 100.784 | 1.00 | 36.29 |
| ATOM | 707 | ND2 | ASN | A | 87 | 39.675 | -0.320 | 102.640 | 1.00 | 45.25 |
| ATOM | 708 | C | ASN | A | 87 | 38.855 | -3.956 | 103.217 | 1.00 | 34.73 |
| ATOM | 709 | O | ASN | A | 87 | 39.868 | -3.315 | 103.512 | 1.00 | 33.23 |
| ATOM | 710 | N | ILE | A | 88 | 38.687 | -5.237 | 103.523 | 1.00 | 32.48 |
| ATOM | 711 | CA | ILE | A | 88 | 39.676 | -6.018 | 104.248 | 1.00 | 33.65 |
| ATOM | 712 | CB | ILE | A | 88 | 39.030 | -6.732 | 105.445 | 1.00 | 38.66 |
| ATOM | 713 | CG2 | ILE | A | 88 | 40.021 | -7.680 | 106.081 | 1.00 | 41.31 |
| ATOM | 714 | CG1 | ILE | A | 88 | 38.536 | -5.707 | 106.461 | 1.00 | 40.45 |
| ATOM | 715 | CD1 | ILE | A | 88 | 39.641 | -4.953 | 107.124 | 1.00 | 42.25 |
| ATOM | 716 | C | ILE | A | 88 | 40.251 | -7.090 | 103.318 | 1.00 | 37.36 |
| ATOM | 717 | O | ILE | A | 88 | 39.555 | -7.587 | 102.431 | 1.00 | 35.47 |
| ATOM | 718 | N | GLY | A | 89 | 41.517 | -7.446 | 103.520 | 1.00 | 31.52 |
| ATOM | 719 | CA | GLY | A | 89 | 42.124 | -8.477 | 102.698 | 1.00 | 33.53 |
| ATOM | 720 | C | GLY | A | 89 | 43.134 | -7.994 | 101.675 | 1.00 | 34.50 |
| ATOM | 721 | O | GLY | A | 89 | 43.951 | -8.777 | 101.186 | 1.00 | 32.81 |
| ATOM | 722 | N | GLY | A | 90 | 43.071 | -6.710 | 101.335 | 1.00 | 31.39 |
| ATOM | 723 | CA | GLY | A | 90 | 44.005 | -6.158 | 100.371 | 1.00 | 23.90 |
| ATOM | 724 | C | GLY | A | 90 | 45.340 | -5.893 | 101.040 | 1.00 | 28.78 |
| ATOM | 725 | O | GLY | A | 90 | 45.563 | -6.339 | 102.163 | 1.00 | 21.71 |
| ATOM | 726 | N | TYR | A | 91 | 46.221 | -5.155 | 100.367 | 1.00 | 28.26 |

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Figure 18-12

| | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|---------|------|-------|
| ATOM | 727 | CA | TYR | A | 91 | 47.539 | -4.850 | 100.918 | 1.00 | 27.34 |
| ATOM | 728 | CB | TYR | A | 91 | 48.477 | -4.365 | 99.805 | 1.00 | 22.62 |
| ATOM | 729 | CG | TYR | A | 91 | 48.066 | -3.039 | 99.194 | 1.00 | 24.28 |
| ATOM | 730 | CD1 | TYR | A | 91 | 48.374 | -1.829 | 99.822 | 1.00 | 21.55 |
| ATOM | 731 | CE1 | TYR | A | 91 | 47.970 | -0.609 | 99.275 | 1.00 | 24.69 |
| ATOM | 732 | CD2 | TYR | A | 91 | 47.341 | -2.997 | 98.002 | 1.00 | 24.86 |
| ATOM | 733 | CE2 | TYR | A | 91 | 46.931 | -1.786 | 97.447 | 1.00 | 29.92 |
| ATOM | 734 | CZ | TYR | A | 91 | 47.250 | -0.597 | 98.086 | 1.00 | 29.04 |
| ATOM | 735 | OH | TYR | A | 91 | 46.861 | 0.593 | 97.516 | 1.00 | 29.51 |
| ATOM | 736 | C | TYR | A | 91 | 47.452 | -3.777 | 101.998 | 1.00 | 27.52 |
| ATOM | 737 | O | TYR | A | 91 | 48.314 | -3.689 | 102.869 | 1.00 | 27.20 |
| ATOM | 738 | N | GLU | A | 92 | 46.402 | -2.971 | 101.938 | 1.00 | 26.75 |
| ATOM | 739 | CA | GLU | A | 92 | 46.232 | -1.879 | 102.882 | 1.00 | 28.38 |
| ATOM | 740 | CB | GLU | A | 92 | 45.234 | -0.881 | 102.310 | 1.00 | 28.57 |
| ATOM | 741 | CG | GLU | A | 92 | 45.232 | 0.471 | 102.982 | 1.00 | 36.94 |
| ATOM | 742 | CD | GLU | A | 92 | 44.178 | 1.395 | 102.396 | 1.00 | 37.40 |
| ATOM | 743 | OE1 | GLU | A | 92 | 42.999 | 1.293 | 102.794 | 1.00 | 31.22 |
| ATOM | 744 | OE2 | GLU | A | 92 | 44.527 | 2.209 | 101.516 | 1.00 | 40.54 |
| ATOM | 745 | C | GLU | A | 92 | 45.770 | -2.343 | 104.259 | 1.00 | 29.20 |
| ATOM | 746 | O | GLU | A | 92 | 46.389 | -2.015 | 105.268 | 1.00 | 21.86 |
| ATOM | 747 | N | ASN | A | 93 | 44.687 | -3.117 | 104.286 | 1.00 | 26.51 |
| ATOM | 748 | CA | ASN | A | 93 | 44.109 | -3.613 | 105.527 | 1.00 | 24.02 |
| ATOM | 749 | CB | ASN | A | 93 | 42.727 | -2.988 | 105.690 | 1.00 | 24.51 |
| ATOM | 750 | CG | ASN | A | 93 | 42.738 | -1.488 | 105.405 | 1.00 | 28.61 |
| ATOM | 751 | OD1 | ASN | A | 93 | 43.428 | -0.727 | 106.079 | 1.00 | 25.30 |
| ATOM | 752 | ND2 | ASN | A | 93 | 41.987 | -1.063 | 104.393 | 1.00 | 20.45 |
| ATOM | 753 | C | ASN | A | 93 | 43.999 | -5.132 | 105.407 | 1.00 | 24.79 |
| ATOM | 754 | O | ASN | A | 93 | 42.905 | -5.680 | 105.291 | 1.00 | 21.89 |
| ATOM | 755 | N | PRO | A | 94 | 45.142 | -5.828 | 105.429 | 1.00 | 24.60 |
| ATOM | 756 | CD | PRO | A | 94 | 46.493 | -5.246 | 105.540 | 1.00 | 22.93 |
| ATOM | 757 | CA | PRO | A | 94 | 45.241 | -7.285 | 105.312 | 1.00 | 27.23 |
| ATOM | 758 | CB | PRO | A | 94 | 46.730 | -7.488 | 105.093 | 1.00 | 25.46 |
| ATOM | 759 | CG | PRO | A | 94 | 47.299 | -6.431 | 106.046 | 1.00 | 26.20 |
| ATOM | 760 | C | PRO | A | 94 | 44.743 | -8.112 | 106.489 | 1.00 | 31.04 |
| ATOM | 761 | O | PRO | A | 94 | 44.411 | -7.589 | 107.558 | 1.00 | 29.10 |
| ATOM | 762 | N | VAL | A | 95 | 44.696 | -9.422 | 106.266 | 1.00 | 28.27 |
| ATOM | 763 | CA | VAL | A | 95 | 44.299 | -10.367 | 107.291 | 1.00 | 28.82 |
| ATOM | 764 | CB | VAL | A | 95 | 43.938 | -11.737 | 106.677 | 1.00 | 30.75 |
| ATOM | 765 | CG1 | VAL | A | 95 | 43.745 | -12.766 | 107.776 | 1.00 | 33.60 |
| ATOM | 766 | CG2 | VAL | A | 95 | 42.679 | -11.611 | 105.849 | 1.00 | 24.87 |
| ATOM | 767 | C | VAL | A | 95 | 45.503 | -10.549 | 108.204 | 1.00 | 29.98 |
| ATOM | 768 | O | VAL | A | 95 | 46.637 | -10.649 | 107.729 | 1.00 | 31.36 |
| ATOM | 769 | N | SER | A | 96 | 45.264 | -10.572 | 109.510 | 1.00 | 29.38 |
| ATOM | 770 | CA | SER | A | 96 | 46.335 | -10.766 | 110.485 | 1.00 | 32.56 |
| ATOM | 771 | CB | SER | A | 96 | 47.325 | -9.600 | 110.454 | 1.00 | 34.15 |
| ATOM | 772 | OG | SER | A | 96 | 46.758 | -8.448 | 111.051 | 1.00 | 28.33 |
| ATOM | 773 | C | SER | A | 96 | 45.681 | -10.804 | 111.854 | 1.00 | 32.10 |
| ATOM | 774 | O | SER | A | 96 | 44.458 | -10.839 | 111.950 | 1.00 | 37.91 |
| ATOM | 775 | N | TYR | A | 97 | 46.484 | -10.795 | 112.913 | 1.00 | 32.57 |
| ATOM | 776 | CA | TYR | A | 97 | 45.914 | -10.801 | 114.248 | 1.00 | 34.95 |
| ATOM | 777 | CB | TYR | A | 97 | 46.685 | -11.735 | 115.182 | 1.00 | 35.47 |
| ATOM | 778 | CG | TYR | A | 97 | 46.492 | -13.187 | 114.817 | 1.00 | 40.65 |
| ATOM | 779 | CD1 | TYR | A | 97 | 47.319 | -13.812 | 113.882 | 1.00 | 40.63 |
| ATOM | 780 | CE1 | TYR | A | 97 | 47.083 | -15.121 | 113.475 | 1.00 | 42.16 |
| ATOM | 781 | CD2 | TYR | A | 97 | 45.421 | -13.910 | 115.338 | 1.00 | 38.82 |
| ATOM | 782 | CE2 | TYR | A | 97 | 45.175 | -15.219 | 114.936 | 1.00 | 42.82 |
| ATOM | 783 | CE | TYR | A | 97 | 46.010 | -15.816 | 114.005 | 1.00 | 42.56 |
| ATOM | 784 | CH | TYR | A | 97 | 45.772 | -17.105 | 113.601 | 1.00 | 46.03 |
| ATOM | 785 | C | TYR | A | 97 | 45.862 | -9.394 | 114.813 | 1.00 | 37.56 |
| ATOM | 786 | O | TYR | A | 97 | 45.601 | -9.195 | 115.998 | 1.00 | 39.06 |
| ATOM | 787 | N | ALA | A | 98 | 46.115 | -8.418 | 113.948 | 1.00 | 31.96 |
| ATOM | 788 | CA | ALA | A | 98 | 46.048 | -7.024 | 114.341 | 1.00 | 30.43 |
| ATOM | 789 | CB | ALA | A | 98 | 47.105 | -6.211 | 113.600 | 1.00 | 29.64 |
| ATOM | 790 | C | ALA | A | 98 | 44.658 | -6.533 | 113.962 | 1.00 | 30.35 |
| ATOM | 791 | O | ALA | A | 98 | 44.099 | -5.655 | 114.612 | 1.00 | 31.82 |
| ATOM | 792 | N | MET | A | 99 | 44.094 | -7.130 | 112.915 | 1.00 | 30.40 |

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Figure 18-13

| | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|---------|---------|------|-------|
| ATOM | 793 | CA | MET | A | 99 | 42.788 | -6.730 | 112.420 | 1.00 | 27.54 |
| ATOM | 794 | CB | MET | A | 99 | 42.370 | -7.620 | 111.238 | 1.00 | 30.55 |
| ATOM | 795 | CG | MET | A | 99 | 42.052 | -9.071 | 111.565 | 1.00 | 31.59 |
| ATOM | 796 | SD | MET | A | 99 | 41.902 | -10.077 | 110.053 | 1.00 | 30.13 |
| ATOM | 797 | CE | MET | A | 99 | 40.770 | -9.086 | 109.085 | 1.00 | 28.02 |
| ATOM | 798 | C | MET | A | 99 | 41.703 | -6.696 | 113.490 | 1.00 | 28.02 |
| ATOM | 799 | O | MET | A | 99 | 40.818 | -5.842 | 113.446 | 1.00 | 24.53 |
| ATOM | 800 | N | PHE | A | 100 | 41.752 | -7.614 | 114.449 | 1.00 | 26.07 |
| ATOM | 801 | CA | PHE | A | 100 | 40.759 | -7.583 | 115.516 | 1.00 | 30.47 |
| ATOM | 802 | CB | PHE | A | 100 | 39.738 | -8.718 | 115.404 | 1.00 | 30.29 |
| ATOM | 803 | CG | PHE | A | 100 | 38.693 | -8.657 | 116.475 | 1.00 | 29.35 |
| ATOM | 804 | CD1 | PHE | A | 100 | 37.722 | -7.662 | 116.455 | 1.00 | 27.01 |
| ATOM | 805 | CD2 | PHE | A | 100 | 38.756 | -9.506 | 117.575 | 1.00 | 30.68 |
| ATOM | 806 | CE1 | PHE | A | 100 | 36.834 | -7.507 | 117.519 | 1.00 | 31.41 |
| ATOM | 807 | CE2 | PHE | A | 100 | 37.873 | -9.356 | 118.644 | 1.00 | 28.39 |
| ATOM | 808 | CZ | PHE | A | 100 | 36.913 | -8.355 | 118.618 | 1.00 | 24.06 |
| ATOM | 809 | C | PHE | A | 100 | 41.345 | -7.616 | 116.922 | 1.00 | 29.67 |
| ATOM | 810 | O | PHE | A | 100 | 41.028 | -6.751 | 117.740 | 1.00 | 29.67 |
| ATOM | 811 | N | THR | A | 101 | 42.181 | -8.610 | 117.222 | 1.00 | 31.30 |
| ATOM | 812 | CA | THR | A | 101 | 42.770 | -8.701 | 118.562 | 1.00 | 31.37 |
| ATOM | 813 | CB | THR | A | 101 | 43.610 | -9.977 | 118.732 | 1.00 | 31.63 |
| ATOM | 814 | OG1 | THR | A | 101 | 42.777 | -11.119 | 118.532 | 1.00 | 31.64 |
| ATOM | 815 | CG2 | THR | A | 101 | 44.197 | -10.045 | 120.137 | 1.00 | 27.38 |
| ATOM | 816 | C | THR | A | 101 | 43.647 | -7.493 | 118.884 | 1.00 | 31.66 |
| ATOM | 817 | O | THR | A | 101 | 43.502 | -6.875 | 119.942 | 1.00 | 30.71 |
| ATOM | 818 | N | GLY | A | 102 | 44.562 | -7.166 | 117.976 | 1.00 | 27.40 |
| ATOM | 819 | CA | GLY | A | 102 | 45.430 | -6.018 | 118.193 | 1.00 | 27.19 |
| ATOM | 820 | C | GLY | A | 102 | 44.631 | -4.728 | 118.266 | 1.00 | 27.26 |
| ATOM | 821 | O | GLY | A | 102 | 44.785 | -3.940 | 119.201 | 1.00 | 27.68 |
| ATOM | 822 | N | SER | A | 103 | 43.767 | -4.515 | 117.279 | 1.00 | 30.52 |
| ATOM | 823 | CA | SER | A | 103 | 42.941 | -3.314 | 117.216 | 1.00 | 31.91 |
| ATOM | 824 | CB | SER | A | 103 | 42.085 | -3.334 | 115.949 | 1.00 | 34.63 |
| ATOM | 825 | OG | SER | A | 103 | 42.896 | -3.265 | 114.791 | 1.00 | 35.94 |
| ATOM | 826 | C | SER | A | 103 | 42.046 | -3.163 | 118.441 | 1.00 | 32.44 |
| ATOM | 827 | O | SER | A | 103 | 41.891 | -2.065 | 118.984 | 1.00 | 25.78 |
| ATOM | 828 | N | SER | A | 104 | 41.455 | -4.270 | 118.871 | 1.00 | 30.47 |
| ATOM | 829 | CA | SER | A | 104 | 40.584 | -4.251 | 120.038 | 1.00 | 30.22 |
| ATOM | 830 | CB | SER | A | 104 | 39.978 | -5.633 | 120.265 | 1.00 | 23.88 |
| ATOM | 831 | OG | SER | A | 104 | 39.078 | -5.595 | 121.358 | 1.00 | 36.91 |
| ATOM | 832 | C | SER | A | 104 | 41.367 | -3.841 | 121.282 | 1.00 | 28.13 |
| ATOM | 833 | O | SER | A | 104 | 40.872 | -3.098 | 122.130 | 1.00 | 25.16 |
| ATOM | 834 | N | LEU | A | 105 | 42.594 | -4.336 | 121.386 | 1.00 | 29.39 |
| ATOM | 835 | CA | LEU | A | 105 | 43.445 | -4.034 | 122.530 | 1.00 | 29.52 |
| ATOM | 836 | CB | LEU | A | 105 | 44.684 | -4.922 | 122.471 | 1.00 | 32.90 |
| ATOM | 837 | CG | LEU | A | 105 | 45.461 | -5.176 | 123.754 | 1.00 | 40.34 |
| ATOM | 838 | CD1 | LEU | A | 105 | 44.520 | -5.723 | 124.828 | 1.00 | 35.95 |
| ATOM | 839 | CD2 | LEU | A | 105 | 46.582 | -6.178 | 123.462 | 1.00 | 40.23 |
| ATOM | 840 | C | LEU | A | 105 | 43.834 | -2.552 | 122.511 | 1.00 | 32.09 |
| ATOM | 841 | O | LEU | A | 105 | 43.896 | -1.894 | 123.554 | 1.00 | 30.38 |
| ATOM | 842 | N | ALA | A | 106 | 44.081 | -2.029 | 121.314 | 1.00 | 30.26 |
| ATOM | 843 | CA | ALA | A | 106 | 44.448 | -0.626 | 121.151 | 1.00 | 28.31 |
| ATOM | 844 | CB | ALA | A | 106 | 44.958 | -0.386 | 119.738 | 1.00 | 23.88 |
| ATOM | 845 | C | ALA | A | 106 | 43.243 | 0.268 | 121.434 | 1.00 | 26.04 |
| ATOM | 846 | O | ALA | A | 106 | 43.380 | 1.376 | 121.952 | 1.00 | 20.63 |
| ATOM | 847 | N | THR | A | 107 | 42.058 | -0.224 | 121.099 | 1.00 | 26.86 |
| ATOM | 848 | CA | THR | A | 107 | 40.841 | 0.542 | 121.322 | 1.00 | 25.04 |
| ATOM | 849 | CB | THR | A | 107 | 39.706 | 0.007 | 120.443 | 1.00 | 26.50 |
| ATOM | 850 | OG1 | THR | A | 107 | 40.111 | 0.092 | 119.069 | 1.00 | 24.62 |
| ATOM | 851 | CG2 | THR | A | 107 | 38.439 | 0.824 | 120.629 | 1.00 | 19.80 |
| ATOM | 852 | C | THR | A | 107 | 40.450 | 0.503 | 122.798 | 1.00 | 27.90 |
| ATOM | 853 | O | THR | A | 107 | 40.039 | 1.515 | 123.361 | 1.00 | 29.04 |
| ATOM | 854 | N | GLY | A | 108 | 40.585 | -0.662 | 123.422 | 1.00 | 24.01 |
| ATOM | 855 | CA | GLY | A | 108 | 40.256 | -0.767 | 124.832 | 1.00 | 24.86 |
| ATOM | 856 | C | GLY | A | 108 | 41.181 | 0.155 | 125.603 | 1.00 | 23.86 |
| ATOM | 857 | O | GLY | A | 108 | 40.771 | 0.790 | 126.572 | 1.00 | 26.97 |
| ATOM | 858 | N | SER | A | 109 | 42.434 | 0.236 | 125.158 | 1.00 | 23.07 |

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Figure 18-14

| | | | | | | | | |
|------|-----|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 859 | CA | SER A 109 | 43.421 | 1.090 | 125.807 | 1.00 | 20.96 |
| ATOM | 860 | CB | SER A 109 | 44.795 | 0.910 | 125.160 | 1.00 | 24.84 |
| ATOM | 861 | OG | SER A 109 | 45.294 | -0.393 | 125.402 | 1.00 | 25.84 |
| ATOM | 862 | C | SER A 109 | 43.008 | 2.552 | 125.759 | 1.00 | 21.13 |
| ATOM | 863 | O | SER A 109 | 43.323 | 3.312 | 126.672 | 1.00 | 23.17 |
| ATOM | 864 | N | THR A 110 | 42.311 | 2.949 | 124.698 | 1.00 | 20.83 |
| ATOM | 865 | CA | THR A 110 | 41.841 | 4.327 | 124.583 | 1.00 | 21.84 |
| ATOM | 866 | CB | THR A 110 | 41.332 | 4.648 | 123.161 | 1.00 | 24.33 |
| ATOM | 867 | OG1 | THR A 110 | 42.452 | 4.769 | 122.276 | 1.00 | 25.38 |
| ATOM | 868 | CG2 | THR A 110 | 40.543 | 5.954 | 123.144 | 1.00 | 21.18 |
| ATOM | 869 | C | THR A 110 | 40.725 | 4.561 | 125.600 | 1.00 | 28.52 |
| ATOM | 870 | O | THR A 110 | 40.632 | 5.637 | 126.197 | 1.00 | 28.27 |
| ATOM | 871 | N | VAL A 111 | 39.882 | 3.558 | 125.809 | 1.00 | 26.88 |
| ATOM | 872 | CA | VAL A 111 | 38.811 | 3.706 | 126.793 | 1.00 | 30.04 |
| ATOM | 873 | CB | VAL A 111 | 37.820 | 2.519 | 126.742 | 1.00 | 29.94 |
| ATOM | 874 | CG1 | VAL A 111 | 36.737 | 2.693 | 127.802 | 1.00 | 27.07 |
| ATOM | 875 | CG2 | VAL A 111 | 37.193 | 2.431 | 125.355 | 1.00 | 25.26 |
| ATOM | 876 | C | VAL A 111 | 39.440 | 3.797 | 128.187 | 1.00 | 28.10 |
| ATOM | 877 | O | VAL A 111 | 38.968 | 4.539 | 129.039 | 1.00 | 26.06 |
| ATOM | 878 | N | GLN A 112 | 40.521 | 3.056 | 128.415 | 1.00 | 23.92 |
| ATOM | 879 | CA | GLN A 112 | 41.188 | 3.097 | 129.711 | 1.00 | 30.27 |
| ATOM | 880 | CB | GLN A 112 | 42.268 | 2.020 | 129.804 | 1.00 | 28.61 |
| ATOM | 881 | CG | GLN A 112 | 41.777 | 0.629 | 129.481 | 1.00 | 28.90 |
| ATOM | 882 | CD | GLN A 112 | 42.883 | -0.397 | 129.564 | 1.00 | 28.60 |
| ATOM | 883 | OE1 | GLN A 112 | 43.344 | -0.740 | 130.653 | 1.00 | 29.68 |
| ATOM | 884 | NE2 | GLN A 112 | 43.333 | -0.880 | 128.409 | 1.00 | 22.13 |
| ATOM | 885 | C | GLN A 112 | 41.834 | 4.461 | 129.931 | 1.00 | 29.99 |
| ATOM | 886 | O | GLN A 112 | 41.791 | 5.006 | 131.035 | 1.00 | 28.43 |
| ATOM | 887 | N | ALA A 113 | 42.453 | 5.004 | 128.885 | 1.00 | 28.64 |
| ATOM | 888 | CA | ALA A 113 | 43.083 | 6.315 | 129.001 | 1.00 | 26.62 |
| ATOM | 889 | CB | ALA A 113 | 43.693 | 6.732 | 127.684 | 1.00 | 23.49 |
| ATOM | 890 | C | ALA A 113 | 42.005 | 7.307 | 129.407 | 1.00 | 24.63 |
| ATOM | 891 | O | ALA A 113 | 42.232 | 8.183 | 130.240 | 1.00 | 26.38 |
| ATOM | 892 | N | ILE A 114 | 40.824 | 7.163 | 128.822 | 1.00 | 25.26 |
| ATOM | 893 | CA | ILE A 114 | 39.728 | 8.063 | 129.145 | 1.00 | 27.05 |
| ATOM | 894 | CB | ILE A 114 | 38.554 | 7.887 | 128.156 | 1.00 | 26.93 |
| ATOM | 895 | CG2 | ILE A 114 | 37.387 | 8.770 | 128.576 | 1.00 | 25.86 |
| ATOM | 896 | CG1 | ILE A 114 | 39.008 | 8.259 | 126.739 | 1.00 | 28.38 |
| ATOM | 897 | CD1 | ILE A 114 | 37.938 | 8.105 | 125.669 | 1.00 | 28.64 |
| ATOM | 898 | C | ILE A 114 | 39.239 | 7.823 | 130.578 | 1.00 | 31.36 |
| ATOM | 899 | O | ILE A 114 | 38.898 | 8.770 | 131.291 | 1.00 | 24.56 |
| ATOM | 900 | N | GLU A 115 | 39.210 | 6.563 | 131.005 | 1.00 | 31.17 |
| ATOM | 901 | CA | GLU A 115 | 38.750 | 6.257 | 132.358 | 1.00 | 32.12 |
| ATOM | 902 | CB | GLU A 115 | 38.729 | 4.744 | 132.607 | 1.00 | 32.15 |
| ATOM | 903 | CG | GLU A 115 | 37.904 | 3.947 | 131.598 | 1.00 | 32.84 |
| ATOM | 904 | CD | GLU A 115 | 37.875 | 2.459 | 131.912 | 1.00 | 34.12 |
| ATOM | 905 | OE1 | GLU A 115 | 38.910 | 1.910 | 132.345 | 1.00 | 30.36 |
| ATOM | 906 | OE2 | GLU A 115 | 36.826 | 1.827 | 131.699 | 1.00 | 31.38 |
| ATOM | 907 | C | GLU A 115 | 39.675 | 6.932 | 133.357 | 1.00 | 31.65 |
| ATOM | 908 | O | GLU A 115 | 39.224 | 7.446 | 134.383 | 1.00 | 29.25 |
| ATOM | 909 | N | GLU A 116 | 40.970 | 6.933 | 133.053 | 1.00 | 31.50 |
| ATOM | 910 | CA | GLU A 116 | 41.942 | 7.564 | 133.934 | 1.00 | 32.34 |
| ATOM | 911 | CB | GLU A 116 | 43.367 | 7.285 | 133.457 | 1.00 | 33.29 |
| ATOM | 912 | CG | GLU A 116 | 43.805 | 5.842 | 133.633 | 1.00 | 32.29 |
| ATOM | 913 | CD | GLU A 116 | 43.701 | 5.378 | 135.079 | 1.00 | 36.87 |
| ATOM | 914 | OE1 | GLU A 116 | 44.329 | 6.003 | 135.961 | 1.00 | 34.07 |
| ATOM | 915 | OE2 | GLU A 116 | 42.993 | 4.385 | 135.335 | 1.00 | 35.00 |
| ATOM | 916 | C | GLU A 116 | 41.702 | 9.067 | 134.006 | 1.00 | 36.69 |
| ATOM | 917 | O | GLU A 116 | 41.863 | 9.678 | 135.066 | 1.00 | 34.39 |
| ATOM | 918 | N | PHE A 117 | 41.317 | 9.661 | 132.881 | 1.00 | 31.19 |
| ATOM | 919 | CA | PHE A 117 | 41.038 | 11.091 | 132.841 | 1.00 | 28.43 |
| ATOM | 920 | CB | PHE A 117 | 40.593 | 11.509 | 131.444 | 1.00 | 30.14 |
| ATOM | 921 | CG | PHE A 117 | 40.044 | 12.908 | 131.381 | 1.00 | 35.78 |
| ATOM | 922 | CD1 | PHE A 117 | 40.882 | 14.006 | 131.501 | 1.00 | 33.39 |
| ATOM | 923 | CD2 | PHE A 117 | 38.675 | 13.123 | 131.225 | 1.00 | 38.90 |
| ATOM | 924 | CE1 | PHE A 117 | 40.372 | 15.299 | 131.466 | 1.00 | 30.65 |

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Figure 18-15

| | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 925 | CE2 | PHE | A | 117 | 38.153 | 14.412 | 131.190 | 1.00 | 36.50 |
| ATOM | 926 | CZ | PHE | A | 117 | 39.003 | 15.501 | 131.310 | 1.00 | 35.41 |
| ATOM | 927 | C | PHE | A | 117 | 39.908 | 11.401 | 133.811 | 1.00 | 32.78 |
| ATOM | 928 | O | PHE | A | 117 | 39.966 | 12.377 | 134.566 | 1.00 | 29.82 |
| ATOM | 929 | N | LEU | A | 118 | 38.874 | 10.568 | 133.771 | 1.00 | 28.61 |
| ATOM | 930 | CA | LEU | A | 118 | 37.720 | 10.751 | 134.632 | 1.00 | 32.00 |
| ATOM | 931 | CB | LEU | A | 118 | 36.621 | 9.748 | 134.263 | 1.00 | 29.19 |
| ATOM | 932 | CG | LEU | A | 118 | 36.098 | 9.830 | 132.820 | 1.00 | 34.47 |
| ATOM | 933 | CD1 | LEU | A | 118 | 34.962 | 8.836 | 132.622 | 1.00 | 32.69 |
| ATOM | 934 | CD2 | LEU | A | 118 | 35.612 | 11.240 | 132.522 | 1.00 | 32.24 |
| ATOM | 935 | C | LEU | A | 118 | 38.123 | 10.590 | 136.094 | 1.00 | 31.17 |
| ATOM | 936 | O | LEU | A | 118 | 37.576 | 11.260 | 136.964 | 1.00 | 28.32 |
| ATOM | 937 | N | LYS | A | 119 | 39.083 | 9.707 | 136.363 | 1.00 | 27.23 |
| ATOM | 938 | CA | LYS | A | 119 | 39.531 | 9.497 | 137.733 | 1.00 | 30.95 |
| ATOM | 939 | CB | LYS | A | 119 | 40.203 | 8.130 | 137.884 | 1.00 | 26.35 |
| ATOM | 940 | CG | LYS | A | 119 | 39.293 | 6.954 | 137.540 | 1.00 | 32.44 |
| ATOM | 941 | CD | LYS | A | 119 | 39.895 | 5.624 | 137.986 | 1.00 | 33.31 |
| ATOM | 942 | CE | LYS | A | 119 | 41.280 | 5.385 | 137.411 | 1.00 | 33.47 |
| ATOM | 943 | NZ | LYS | A | 119 | 41.874 | 4.102 | 137.904 | 1.00 | 33.40 |
| ATOM | 944 | C | LYS | A | 119 | 40.493 | 10.594 | 138.173 | 1.00 | 32.65 |
| ATOM | 945 | O | LYS | A | 119 | 41.050 | 10.548 | 139.270 | 1.00 | 28.83 |
| ATOM | 946 | N | GLY | A | 120 | 40.689 | 11.583 | 137.308 | 1.00 | 33.77 |
| ATOM | 947 | CA | GLY | A | 120 | 41.571 | 12.677 | 137.652 | 1.00 | 33.84 |
| ATOM | 948 | C | GLY | A | 120 | 43.035 | 12.448 | 137.340 | 1.00 | 34.27 |
| ATOM | 949 | O | GLY | A | 120 | 43.880 | 13.227 | 137.776 | 1.00 | 36.80 |
| ATOM | 950 | N | ASN | A | 121 | 43.347 | 11.384 | 136.606 | 1.00 | 30.77 |
| ATOM | 951 | CA | ASN | A | 121 | 44.731 | 11.122 | 136.244 | 1.00 | 31.73 |
| ATOM | 952 | CB | ASN | A | 121 | 45.089 | 9.646 | 136.437 | 1.00 | 29.34 |
| ATOM | 953 | CG | ASN | A | 121 | 44.856 | 9.170 | 137.851 | 1.00 | 35.83 |
| ATOM | 954 | OD1 | ASN | A | 121 | 45.190 | 9.861 | 138.816 | 1.00 | 32.74 |
| ATOM | 955 | ND2 | ASN | A | 121 | 44.304 | 7.970 | 137.986 | 1.00 | 33.20 |
| ATOM | 956 | C | ASN | A | 121 | 44.954 | 11.506 | 134.790 | 1.00 | 32.59 |
| ATOM | 957 | O | ASN | A | 121 | 44.031 | 11.952 | 134.110 | 1.00 | 34.69 |
| ATOM | 958 | N | VAL | A | 122 | 46.186 | 11.334 | 134.322 | 1.00 | 32.74 |
| ATOM | 959 | CA | VAL | A | 122 | 46.540 | 11.653 | 132.946 | 1.00 | 33.59 |
| ATOM | 960 | CB | VAL | A | 122 | 47.571 | 12.790 | 132.882 | 1.00 | 36.05 |
| ATOM | 961 | CG1 | VAL | A | 122 | 47.884 | 13.121 | 131.438 | 1.00 | 37.58 |
| ATOM | 962 | CG2 | VAL | A | 122 | 47.029 | 14.021 | 133.602 | 1.00 | 37.19 |
| ATOM | 963 | C | VAL | A | 122 | 47.147 | 10.397 | 132.352 | 1.00 | 34.47 |
| ATOM | 964 | O | VAL | A | 122 | 48.053 | 9.801 | 132.939 | 1.00 | 31.28 |
| ATOM | 965 | N | ALA | A | 123 | 46.646 | 9.989 | 131.196 | 1.00 | 28.06 |
| ATOM | 966 | CA | ALA | A | 123 | 47.142 | 8.784 | 130.563 | 1.00 | 30.73 |
| ATOM | 967 | CB | ALA | A | 123 | 46.133 | 7.666 | 130.727 | 1.00 | 32.69 |
| ATOM | 968 | C | ALA | A | 123 | 47.466 | 8.969 | 129.088 | 1.00 | 30.55 |
| ATOM | 969 | O | ALA | A | 123 | 46.909 | 9.830 | 128.406 | 1.00 | 32.89 |
| ATOM | 970 | N | PHE | A | 124 | 48.380 | 8.136 | 128.613 | 1.00 | 27.53 |
| ATOM | 971 | CA | PHE | A | 124 | 48.807 | 8.157 | 127.229 | 1.00 | 26.56 |
| ATOM | 972 | CB | PHE | A | 124 | 50.261 | 8.660 | 127.157 | 1.00 | 25.32 |
| ATOM | 973 | CG | PHE | A | 124 | 50.903 | 8.544 | 125.793 | 1.00 | 27.84 |
| ATOM | 974 | CD1 | PHE | A | 124 | 50.179 | 8.785 | 124.629 | 1.00 | 24.77 |
| ATOM | 975 | CD2 | PHE | A | 124 | 52.266 | 8.266 | 125.686 | 1.00 | 21.79 |
| ATOM | 976 | CE1 | PHE | A | 124 | 50.802 | 8.753 | 123.385 | 1.00 | 29.19 |
| ATOM | 977 | CE2 | PHE | A | 124 | 52.894 | 8.235 | 124.449 | 1.00 | 27.38 |
| ATOM | 978 | CZ | PHE | A | 124 | 52.164 | 8.478 | 123.296 | 1.00 | 20.91 |
| ATOM | 979 | C | PHE | A | 124 | 48.671 | 6.749 | 126.675 | 1.00 | 21.13 |
| ATOM | 980 | O | PHE | A | 124 | 49.181 | 5.795 | 127.260 | 1.00 | 25.38 |
| ATOM | 981 | N | ASN | A | 125 | 47.933 | 6.624 | 125.580 | 1.00 | 18.87 |
| ATOM | 982 | CA | ASN | A | 125 | 47.750 | 5.342 | 124.905 | 1.00 | 25.05 |
| ATOM | 983 | CB | ASN | A | 125 | 46.271 | 4.982 | 124.756 | 1.00 | 22.99 |
| ATOM | 984 | CG | ASN | A | 125 | 46.073 | 3.784 | 123.856 | 1.00 | 24.08 |
| ATOM | 985 | OD1 | ASN | A | 125 | 46.916 | 2.888 | 123.822 | 1.00 | 20.46 |
| ATOM | 986 | ND2 | ASN | A | 125 | 44.960 | 3.748 | 123.138 | 1.00 | 16.10 |
| ATOM | 987 | C | ASN | A | 125 | 48.380 | 5.410 | 123.518 | 1.00 | 23.43 |
| ATOM | 988 | O | ASN | A | 125 | 47.718 | 5.749 | 122.542 | 1.00 | 23.48 |
| ATOM | 989 | N | PRO | A | 126 | 49.680 | 5.103 | 123.423 | 1.00 | 24.55 |
| ATOM | 990 | CD | PRO | A | 126 | 50.589 | 4.730 | 124.519 | 1.00 | 22.87 |

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Figure 18-16

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 991 | CA | PRO A 126 | 50.413 | 5.130 | 122.160 | 1.00 | 22.39 |
| ATOM | 992 | CB | PRO A 126 | 51.829 | 4.751 | 122.594 | 1.00 | 18.20 |
| ATOM | 993 | CG | PRO A 126 | 51.564 | 3.849 | 123.798 | 1.00 | 25.43 |
| ATOM | 994 | C | PRO A 126 | 49.867 | 4.224 | 121.058 | 1.00 | 23.18 |
| ATOM | 995 | O | PRO A 126 | 50.173 | 4.436 | 119.893 | 1.00 | 20.12 |
| ATOM | 996 | N | ALA A 127 | 49.058 | 3.232 | 121.423 | 1.00 | 23.27 |
| ATOM | 997 | CA | ALA A 127 | 48.493 | 2.306 | 120.444 | 1.00 | 23.89 |
| ATOM | 998 | CB | ALA A 127 | 48.176 | 0.967 | 121.118 | 1.00 | 24.82 |
| ATOM | 999 | C | ALA A 127 | 47.241 | 2.864 | 119.778 | 1.00 | 24.76 |
| ATOM | 1000 | O | ALA A 127 | 46.806 | 2.360 | 118.745 | 1.00 | 28.99 |
| ATOM | 1001 | N | GLY A 128 | 46.666 | 3.906 | 120.367 | 1.00 | 22.12 |
| ATOM | 1002 | CA | GLY A 128 | 45.461 | 4.494 | 119.809 | 1.00 | 21.43 |
| ATOM | 1003 | C | GLY A 128 | 45.732 | 5.521 | 118.725 | 1.00 | 23.55 |
| ATOM | 1004 | O | GLY A 128 | 46.875 | 5.695 | 118.291 | 1.00 | 23.25 |
| ATOM | 1005 | N | GLY A 129 | 44.680 | 6.199 | 118.283 | 1.00 | 18.03 |
| ATOM | 1006 | CA | GLY A 129 | 44.822 | 7.205 | 117.243 | 1.00 | 24.99 |
| ATOM | 1007 | C | GLY A 129 | 44.600 | 6.655 | 115.847 | 1.00 | 25.11 |
| ATOM | 1008 | O | GLY A 129 | 44.963 | 7.293 | 114.857 | 1.00 | 24.99 |
| ATOM | 1009 | N | MET A 130 | 44.002 | 5.470 | 115.765 | 1.00 | 20.01 |
| ATOM | 1010 | CA | MET A 130 | 43.729 | 4.825 | 114.481 | 1.00 | 23.63 |
| ATOM | 1011 | CB | MET A 130 | 43.360 | 3.361 | 114.744 | 1.00 | 22.77 |
| ATOM | 1012 | CG | MET A 130 | 44.455 | 2.661 | 115.563 | 1.00 | 26.30 |
| ATOM | 1013 | SD | MET A 130 | 44.198 | 0.913 | 115.989 | 1.00 | 26.57 |
| ATOM | 1014 | CE | MET A 130 | 42.665 | 1.030 | 116.936 | 1.00 | 27.59 |
| ATOM | 1015 | C | MET A 130 | 42.580 | 5.617 | 113.869 | 1.00 | 23.70 |
| ATOM | 1016 | O | MET A 130 | 41.421 | 5.199 | 113.901 | 1.00 | 26.28 |
| ATOM | 1017 | N | HIS A 131 | 42.926 | 6.766 | 113.294 | 1.00 | 20.66 |
| ATOM | 1018 | CA | HIS A 131 | 41.933 | 7.687 | 112.775 | 1.00 | 20.99 |
| ATOM | 1019 | CB | HIS A 131 | 42.474 | 9.125 | 112.891 | 1.00 | 21.01 |
| ATOM | 1020 | CG | HIS A 131 | 43.699 | 9.391 | 112.069 | 1.00 | 28.30 |
| ATOM | 1021 | CD2 | HIS A 131 | 44.498 | 8.549 | 111.373 | 1.00 | 19.65 |
| ATOM | 1022 | ND1 | HIS A 131 | 44.246 | 10.649 | 111.917 | 1.00 | 27.76 |
| ATOM | 1023 | CE1 | HIS A 131 | 45.328 | 10.567 | 111.163 | 1.00 | 20.48 |
| ATOM | 1024 | NE2 | HIS A 131 | 45.503 | 9.302 | 110.820 | 1.00 | 24.18 |
| ATOM | 1025 | C | HIS A 131 | 41.280 | 7.513 | 111.416 | 1.00 | 23.76 |
| ATOM | 1026 | O | HIS A 131 | 40.453 | 8.341 | 111.051 | 1.00 | 21.95 |
| ATOM | 1027 | N | HIS A 132 | 41.600 | 6.449 | 110.682 | 1.00 | 25.12 |
| ATOM | 1028 | CA | HIS A 132 | 41.006 | 6.257 | 109.354 | 1.00 | 23.32 |
| ATOM | 1029 | CB | HIS A 132 | 42.060 | 5.715 | 108.388 | 1.00 | 17.87 |
| ATOM | 1030 | CG | HIS A 132 | 43.148 | 6.689 | 108.072 | 1.00 | 24.79 |
| ATOM | 1031 | CD2 | HIS A 132 | 44.496 | 6.574 | 108.144 | 1.00 | 21.72 |
| ATOM | 1032 | ND1 | HIS A 132 | 42.896 | 7.944 | 107.556 | 1.00 | 13.58 |
| ATOM | 1033 | CE1 | HIS A 132 | 44.044 | 8.558 | 107.323 | 1.00 | 15.41 |
| ATOM | 1034 | NE2 | HIS A 132 | 45.028 | 7.748 | 107.668 | 1.00 | 15.27 |
| ATOM | 1035 | C | HIS A 132 | 39.752 | 5.386 | 109.208 | 1.00 | 23.38 |
| ATOM | 1036 | O | HIS A 132 | 38.947 | 5.615 | 108.304 | 1.00 | 24.70 |
| ATOM | 1037 | N | ALA A 133 | 39.587 | 4.388 | 110.070 | 1.00 | 23.34 |
| ATOM | 1038 | CA | ALA A 133 | 38.453 | 3.471 | 109.953 | 1.00 | 23.77 |
| ATOM | 1039 | CB | ALA A 133 | 38.515 | 2.417 | 111.053 | 1.00 | 27.49 |
| ATOM | 1040 | C | ALA A 133 | 37.093 | 4.145 | 109.966 | 1.00 | 23.02 |
| ATOM | 1041 | O | ALA A 133 | 36.878 | 5.117 | 110.691 | 1.00 | 25.98 |
| ATOM | 1042 | N | PHE A 134 | 36.179 | 3.633 | 109.148 | 1.00 | 18.90 |
| ATOM | 1043 | CA | PHE A 134 | 34.831 | 4.173 | 109.103 | 1.00 | 23.73 |
| ATOM | 1044 | CB | PHE A 134 | 34.317 | 4.296 | 107.663 | 1.00 | 24.29 |
| ATOM | 1045 | CG | PHE A 134 | 35.119 | 5.225 | 106.801 | 1.00 | 26.67 |
| ATOM | 1046 | CD1 | PHE A 134 | 36.025 | 4.724 | 105.867 | 1.00 | 28.69 |
| ATOM | 1047 | CD2 | PHE A 134 | 34.975 | 6.605 | 106.921 | 1.00 | 32.49 |
| ATOM | 1048 | CE1 | PHE A 134 | 36.775 | 5.582 | 105.063 | 1.00 | 28.65 |
| ATOM | 1049 | CE2 | PHE A 134 | 35.724 | 7.479 | 106.119 | 1.00 | 27.86 |
| ATOM | 1050 | CZ | PHE A 134 | 36.623 | 6.967 | 105.188 | 1.00 | 23.93 |
| ATOM | 1051 | C | PHE A 134 | 33.894 | 3.260 | 109.884 | 1.00 | 25.91 |
| ATOM | 1052 | O | PHE A 134 | 34.270 | 2.172 | 110.319 | 1.00 | 27.20 |
| ATOM | 1053 | N | LYS A 135 | 32.670 | 3.728 | 110.062 | 1.00 | 29.14 |
| ATOM | 1054 | CA | LYS A 135 | 31.638 | 2.984 | 110.765 | 1.00 | 35.26 |
| ATOM | 1055 | CB | LYS A 135 | 30.294 | 3.628 | 110.429 | 1.00 | 35.86 |
| ATOM | 1056 | CG | LYS A 135 | 29.072 | 2.779 | 110.667 | 1.00 | 46.26 |

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Figure 18-17

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1057 | CD | LYS | A | 135 | 27.834 | 3.542 | 110.211 | 1.00 | 47.72 |
| ATOM | 1058 | CE | LYS | A | 135 | 26.610 | 2.645 | 110.169 | 1.00 | 53.65 |
| ATOM | 1059 | NZ | LYS | A | 135 | 26.788 | 1.549 | 109.167 | 1.00 | 53.27 |
| ATOM | 1060 | C | LYS | A | 135 | 31.617 | 1.490 | 110.414 | 1.00 | 35.62 |
| ATOM | 1061 | O | LYS | A | 135 | 31.609 | 0.635 | 111.301 | 1.00 | 32.58 |
| ATOM | 1062 | N | SER | A | 136 | 31.629 | 1.180 | 109.122 | 1.00 | 35.97 |
| ATOM | 1063 | CA | SER | A | 136 | 31.555 | -0.211 | 108.684 | 1.00 | 38.99 |
| ATOM | 1064 | CB | SER | A | 136 | 30.172 | -0.474 | 108.083 | 1.00 | 38.87 |
| ATOM | 1065 | OG | SER | A | 136 | 29.146 | -0.072 | 108.975 | 1.00 | 43.54 |
| ATOM | 1066 | C | SER | A | 136 | 32.608 | -0.616 | 107.660 | 1.00 | 37.84 |
| ATOM | 1067 | O | SER | A | 136 | 32.350 | -1.491 | 106.828 | 1.00 | 36.33 |
| ATOM | 1068 | N | ARG | A | 137 | 33.788 | -0.008 | 107.705 | 1.00 | 33.23 |
| ATOM | 1069 | CA | ARG | A | 137 | 34.797 | -0.368 | 106.724 | 1.00 | 30.89 |
| ATOM | 1070 | CB | ARG | A | 137 | 34.456 | 0.291 | 105.385 | 1.00 | 33.88 |
| ATOM | 1071 | CG | ARG | A | 137 | 35.009 | -0.465 | 104.201 | 1.00 | 44.41 |
| ATOM | 1072 | CD | ARG | A | 137 | 34.809 | 0.261 | 102.880 | 1.00 | 46.27 |
| ATOM | 1073 | NE | ARG | A | 137 | 35.091 | -0.645 | 101.768 | 1.00 | 48.87 |
| ATOM | 1074 | CZ | ARG | A | 137 | 35.352 | -0.261 | 100.526 | 1.00 | 48.64 |
| ATOM | 1075 | NH1 | ARG | A | 137 | 35.372 | 1.029 | 100.220 | 1.00 | 51.82 |
| ATOM | 1076 | NH2 | ARG | A | 137 | 35.592 | -1.169 | 99.589 | 1.00 | 49.01 |
| ATOM | 1077 | C | ARG | A | 137 | 36.209 | 0.021 | 107.143 | 1.00 | 31.84 |
| ATOM | 1078 | O | ARG | A | 137 | 36.428 | 1.079 | 107.742 | 1.00 | 30.36 |
| ATOM | 1079 | N | ALA | A | 138 | 37.166 | -0.845 | 106.828 | 1.00 | 30.06 |
| ATOM | 1080 | CA | ALA | A | 138 | 38.560 | -0.588 | 107.158 | 1.00 | 32.24 |
| ATOM | 1081 | CB | ALA | A | 138 | 39.367 | -1.864 | 107.048 | 1.00 | 31.25 |
| ATOM | 1082 | C | ALA | A | 138 | 39.095 | 0.449 | 106.187 | 1.00 | 29.49 |
| ATOM | 1083 | O | ALA | A | 138 | 38.612 | 0.551 | 105.063 | 1.00 | 26.11 |
| ATOM | 1084 | N | ASN | A | 139 | 40.099 | 1.206 | 106.615 | 1.00 | 29.54 |
| ATOM | 1085 | CA | ASN | A | 139 | 40.673 | 2.241 | 105.767 | 1.00 | 26.99 |
| ATOM | 1086 | CB | ASN | A | 139 | 39.685 | 3.415 | 105.662 | 1.00 | 24.10 |
| ATOM | 1087 | CG | ASN | A | 139 | 40.209 | 4.556 | 104.811 | 1.00 | 28.02 |
| ATOM | 1088 | OD1 | ASN | A | 139 | 40.729 | 4.334 | 103.727 | 1.00 | 26.90 |
| ATOM | 1089 | ND2 | ASN | A | 139 | 40.050 | 5.789 | 105.293 | 1.00 | 23.55 |
| ATOM | 1090 | C | ASN | A | 139 | 42.027 | 2.713 | 106.285 | 1.00 | 30.17 |
| ATOM | 1091 | O | ASN | A | 139 | 42.245 | 2.827 | 107.497 | 1.00 | 27.55 |
| ATOM | 1092 | N | GLY | A | 140 | 42.944 | 2.959 | 105.354 | 1.00 | 31.82 |
| ATOM | 1093 | CA | GLY | A | 140 | 44.277 | 3.428 | 105.702 | 1.00 | 24.90 |
| ATOM | 1094 | C | GLY | A | 140 | 45.000 | 2.696 | 106.816 | 1.00 | 27.79 |
| ATOM | 1095 | O | GLY | A | 140 | 45.560 | 3.339 | 107.705 | 1.00 | 23.85 |
| ATOM | 1096 | N | PHE | A | 141 | 45.006 | 1.365 | 106.768 | 1.00 | 24.35 |
| ATOM | 1097 | CA | PHE | A | 141 | 45.679 | 0.538 | 107.783 | 1.00 | 24.53 |
| ATOM | 1098 | CB | PHE | A | 141 | 47.031 | 1.146 | 108.197 | 1.00 | 26.40 |
| ATOM | 1099 | CG | PHE | A | 141 | 47.997 | 1.366 | 107.062 | 1.00 | 30.31 |
| ATOM | 1100 | CD1 | PHE | A | 141 | 49.145 | 2.125 | 107.269 | 1.00 | 31.60 |
| ATOM | 1101 | CD2 | PHE | A | 141 | 47.781 | 0.811 | 105.802 | 1.00 | 29.44 |
| ATOM | 1102 | CE1 | PHE | A | 141 | 50.066 | 2.331 | 106.243 | 1.00 | 30.44 |
| ATOM | 1103 | CE2 | PHE | A | 141 | 48.694 | 1.008 | 104.770 | 1.00 | 27.91 |
| ATOM | 1104 | CZ | PHE | A | 141 | 49.840 | 1.771 | 104.991 | 1.00 | 29.38 |
| ATOM | 1105 | C | PHE | A | 141 | 44.846 | 0.387 | 109.056 | 1.00 | 23.53 |
| ATOM | 1106 | O | PHE | A | 141 | 45.194 | -0.399 | 109.941 | 1.00 | 23.09 |
| ATOM | 1107 | N | CYS | A | 142 | 43.760 | 1.143 | 109.159 | 1.00 | 22.86 |
| ATOM | 1108 | CA | CYS | A | 142 | 42.925 | 1.099 | 110.356 | 1.00 | 23.87 |
| ATOM | 1109 | CB | CYS | A | 142 | 42.472 | 2.516 | 110.723 | 1.00 | 22.51 |
| ATOM | 1110 | SG | CYS | A | 142 | 43.828 | 3.683 | 111.072 | 1.00 | 27.62 |
| ATOM | 1111 | C | CYS | A | 142 | 41.694 | 0.205 | 110.233 | 1.00 | 24.20 |
| ATOM | 1112 | O | CYS | A | 142 | 40.932 | 0.307 | 109.272 | 1.00 | 24.12 |
| ATOM | 1113 | N | TYR | A | 143 | 41.498 | -0.663 | 111.219 | 1.00 | 23.84 |
| ATOM | 1114 | CA | TYR | A | 143 | 40.335 | -1.546 | 111.236 | 1.00 | 26.07 |
| ATOM | 1115 | CB | TYR | A | 143 | 40.728 | -2.958 | 111.680 | 1.00 | 27.89 |
| ATOM | 1116 | CG | TYR | A | 143 | 41.829 | -3.582 | 110.855 | 1.00 | 27.30 |
| ATOM | 1117 | CD1 | TYR | A | 143 | 43.169 | -3.329 | 111.137 | 1.00 | 25.76 |
| ATOM | 1118 | CE1 | TYR | A | 143 | 44.185 | -3.875 | 110.346 | 1.00 | 25.77 |
| ATOM | 1119 | CD2 | TYR | A | 143 | 41.526 | -4.394 | 109.762 | 1.00 | 25.87 |
| ATOM | 1120 | CE2 | TYR | A | 143 | 42.531 | -4.941 | 108.967 | 1.00 | 23.10 |
| ATOM | 1121 | CZ | TYR | A | 143 | 43.854 | -4.679 | 109.262 | 1.00 | 22.93 |
| ATOM | 1122 | OH | TYR | A | 143 | 44.849 | -5.217 | 108.476 | 1.00 | 20.64 |

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Figure 18-18

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 1123 | C | TYR A 143 | 39.281 | -0.991 | 112.193 | 1.00 | 24.56 |
| ATOM | 1124 | O | TYR A 143 | 38.085 | -1.030 | 111.905 | 1.00 | 24.88 |
| ATOM | 1125 | N | ILE A 144 | 39.734 | -0.471 | 113.331 | 1.00 | 23.77 |
| ATOM | 1126 | CA | ILE A 144 | 38.833 | 0.102 | 114.335 | 1.00 | 27.11 |
| ATOM | 1127 | CB | ILE A 144 | 38.871 | -0.729 | 115.643 | 1.00 | 24.56 |
| ATOM | 1128 | CG2 | ILE A 144 | 37.941 | -0.120 | 116.690 | 1.00 | 23.47 |
| ATOM | 1129 | CG1 | ILE A 144 | 38.430 | -2.169 | 115.346 | 1.00 | 28.51 |
| ATOM | 1130 | CD1 | ILE A 144 | 38.535 | -3.113 | 116.539 | 1.00 | 28.70 |
| ATOM | 1131 | C | ILE A 144 | 39.248 | 1.550 | 114.627 | 1.00 | 24.15 |
| ATOM | 1132 | O | ILE A 144 | 40.428 | 1.843 | 114.800 | 1.00 | 24.42 |
| ATOM | 1133 | N | ASN A 145 | 38.277 | 2.453 | 114.669 | 1.00 | 22.04 |
| ATOM | 1134 | CA | ASN A 145 | 38.555 | 3.866 | 114.920 | 1.00 | 21.31 |
| ATOM | 1135 | CB | ASN A 145 | 37.559 | 4.732 | 114.133 | 1.00 | 18.87 |
| ATOM | 1136 | CG | ASN A 145 | 37.956 | 6.205 | 114.091 | 1.00 | 22.21 |
| ATOM | 1137 | OD1 | ASN A 145 | 38.223 | 6.823 | 115.124 | 1.00 | 22.47 |
| ATOM | 1138 | ND2 | ASN A 145 | 37.978 | 6.776 | 112.892 | 1.00 | 23.78 |
| ATOM | 1139 | C | ASN A 145 | 38.417 | 4.141 | 116.418 | 1.00 | 22.63 |
| ATOM | 1140 | O | ASN A 145 | 37.338 | 4.535 | 116.880 | 1.00 | 22.45 |
| ATOM | 1141 | N | ASN A 146 | 39.495 | 3.941 | 117.178 | 1.00 | 16.63 |
| ATOM | 1142 | CA | ASN A 146 | 39.423 | 4.160 | 118.628 | 1.00 | 23.57 |
| ATOM | 1143 | CB | ASN A 146 | 40.708 | 3.678 | 119.320 | 1.00 | 19.80 |
| ATOM | 1144 | CG | ASN A 146 | 41.924 | 4.508 | 118.967 | 1.00 | 27.81 |
| ATOM | 1145 | OD1 | ASN A 146 | 42.299 | 5.421 | 119.704 | 1.00 | 19.55 |
| ATOM | 1146 | ND2 | ASN A 146 | 42.544 | 4.202 | 117.827 | 1.00 | 19.55 |
| ATOM | 1147 | C | ASN A 146 | 39.079 | 5.602 | 119.023 | 1.00 | 26.32 |
| ATOM | 1148 | O | ASN A 146 | 38.452 | 5.827 | 120.059 | 1.00 | 28.34 |
| ATOM | 1149 | N | PRO A 147 | 39.512 | 6.605 | 118.231 | 1.00 | 28.46 |
| ATOM | 1150 | CD | PRO A 147 | 40.383 | 6.637 | 117.042 | 1.00 | 27.18 |
| ATOM | 1151 | CA | PRO A 147 | 39.150 | 7.972 | 118.618 | 1.00 | 24.15 |
| ATOM | 1152 | CB | PRO A 147 | 39.859 | 8.815 | 117.558 | 1.00 | 25.13 |
| ATOM | 1153 | CG | PRO A 147 | 41.081 | 7.959 | 117.235 | 1.00 | 30.05 |
| ATOM | 1154 | C | PRO A 147 | 37.618 | 8.136 | 118.578 | 1.00 | 26.71 |
| ATOM | 1155 | O | PRO A 147 | 37.017 | 8.760 | 119.456 | 1.00 | 24.93 |
| ATOM | 1156 | N | ALA A 148 | 36.989 | 7.557 | 117.562 | 1.00 | 21.42 |
| ATOM | 1157 | CA | ALA A 148 | 35.536 | 7.633 | 117.416 | 1.00 | 21.03 |
| ATOM | 1158 | CB | ALA A 148 | 35.112 | 7.044 | 116.072 | 1.00 | 19.98 |
| ATOM | 1159 | C | ALA A 148 | 34.838 | 6.891 | 118.552 | 1.00 | 20.49 |
| ATOM | 1160 | O | ALA A 148 | 33.822 | 7.344 | 119.067 | 1.00 | 21.44 |
| ATOM | 1161 | N | VAL A 149 | 35.381 | 5.739 | 118.928 | 1.00 | 19.20 |
| ATOM | 1162 | CA | VAL A 149 | 34.818 | 4.950 | 120.016 | 1.00 | 24.61 |
| ATOM | 1163 | CB | VAL A 149 | 35.570 | 3.608 | 120.181 | 1.00 | 25.96 |
| ATOM | 1164 | CG1 | VAL A 149 | 35.158 | 2.918 | 121.485 | 1.00 | 26.58 |
| ATOM | 1165 | CG2 | VAL A 149 | 35.262 | 2.704 | 118.995 | 1.00 | 25.67 |
| ATOM | 1166 | C | VAL A 149 | 34.947 | 5.752 | 121.304 | 1.00 | 23.56 |
| ATOM | 1167 | O | VAL A 149 | 33.990 | 5.887 | 122.064 | 1.00 | 22.52 |
| ATOM | 1168 | N | GLY A 150 | 36.143 | 6.287 | 121.536 | 1.00 | 24.65 |
| ATOM | 1169 | CA | GLY A 150 | 36.390 | 7.074 | 122.731 | 1.00 | 22.82 |
| ATOM | 1170 | C | GLY A 150 | 35.477 | 8.281 | 122.838 | 1.00 | 25.46 |
| ATOM | 1171 | O | GLY A 150 | 34.919 | 8.564 | 123.904 | 1.00 | 23.17 |
| ATOM | 1172 | N | ILE A 151 | 35.327 | 9.001 | 121.733 | 1.00 | 24.38 |
| ATOM | 1173 | CA | ILE A 151 | 34.481 | 10.180 | 121.716 | 1.00 | 22.85 |
| ATOM | 1174 | CB | ILE A 151 | 34.610 | 10.928 | 120.371 | 1.00 | 24.45 |
| ATOM | 1175 | CG2 | ILE A 151 | 33.598 | 12.077 | 120.306 | 1.00 | 24.71 |
| ATOM | 1176 | CG1 | ILE A 151 | 36.041 | 11.462 | 120.222 | 1.00 | 28.02 |
| ATOM | 1177 | CD1 | ILE A 151 | 36.354 | 12.056 | 118.854 | 1.00 | 27.10 |
| ATOM | 1178 | C | ILE A 151 | 33.018 | 9.806 | 121.987 | 1.00 | 28.19 |
| ATOM | 1179 | O | ILE A 151 | 32.337 | 10.482 | 122.763 | 1.00 | 26.37 |
| ATOM | 1180 | N | GLU A 152 | 32.532 | 8.734 | 121.364 | 1.00 | 26.32 |
| ATOM | 1181 | CA | GLU A 152 | 31.149 | 8.314 | 121.601 | 1.00 | 30.07 |
| ATOM | 1182 | CB | GLU A 152 | 30.758 | 7.161 | 120.672 | 1.00 | 29.37 |
| ATOM | 1183 | CG | GLU A 152 | 30.609 | 7.543 | 119.194 | 1.00 | 27.68 |
| ATOM | 1184 | CD | GLU A 152 | 29.455 | 8.504 | 118.946 | 1.00 | 31.82 |
| ATOM | 1185 | OE1 | GLU A 152 | 29.139 | 8.777 | 117.773 | 1.00 | 33.51 |
| ATOM | 1186 | OE2 | GLU A 152 | 28.862 | 9.009 | 119.918 | 1.00 | 34.73 |
| ATOM | 1187 | C | GLU A 152 | 31.009 | 7.879 | 123.055 | 1.00 | 28.00 |
| ATOM | 1188 | O | GLU A 152 | 29.980 | 8.096 | 123.683 | 1.00 | 31.23 |

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Figure 18-19

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1189 | N | TYR | A | 153 | 32.054 | 7.253 | 123.583 | 1.00 | 28.72 |
| ATOM | 1190 | CA | TYR | A | 153 | 32.066 | 6.805 | 124.971 | 1.00 | 31.35 |
| ATOM | 1191 | CB | TYR | A | 153 | 33.427 | 6.204 | 125.307 | 1.00 | 31.56 |
| ATOM | 1192 | CG | TYR | A | 153 | 33.617 | 5.839 | 126.759 | 1.00 | 33.17 |
| ATOM | 1193 | CD1 | TYR | A | 153 | 33.111 | 4.647 | 127.280 | 1.00 | 35.43 |
| ATOM | 1194 | CE1 | TYR | A | 153 | 33.321 | 4.298 | 128.619 | 1.00 | 33.52 |
| ATOM | 1195 | CD2 | TYR | A | 153 | 34.329 | 6.677 | 127.611 | 1.00 | 34.29 |
| ATOM | 1196 | CE2 | TYR | A | 153 | 34.544 | 6.342 | 128.944 | 1.00 | 35.34 |
| ATOM | 1197 | CZ | TYR | A | 153 | 34.041 | 5.154 | 129.444 | 1.00 | 37.50 |
| ATOM | 1198 | OH | TYR | A | 153 | 34.260 | 4.835 | 130.767 | 1.00 | 30.10 |
| ATOM | 1199 | C | TYR | A | 153 | 31.828 | 8.022 | 125.857 | 1.00 | 32.71 |
| ATOM | 1200 | O | TYR | A | 153 | 31.026 | 7.988 | 126.787 | 1.00 | 29.14 |
| ATOM | 1201 | N | LEU | A | 154 | 32.538 | 9.102 | 125.552 | 1.00 | 29.65 |
| ATOM | 1202 | CA | LEU | A | 154 | 32.413 | 10.332 | 126.310 | 1.00 | 32.87 |
| ATOM | 1203 | CB | LEU | A | 154 | 33.477 | 11.329 | 125.847 | 1.00 | 31.46 |
| ATOM | 1204 | CG | LEU | A | 154 | 34.910 | 11.053 | 126.324 | 1.00 | 29.68 |
| ATOM | 1205 | CD1 | LEU | A | 154 | 35.898 | 11.953 | 125.605 | 1.00 | 29.29 |
| ATOM | 1206 | CD2 | LEU | A | 154 | 34.989 | 11.278 | 127.829 | 1.00 | 27.19 |
| ATOM | 1207 | C | LEU | A | 154 | 31.020 | 10.952 | 126.232 | 1.00 | 34.63 |
| ATOM | 1208 | O | LEU | A | 154 | 30.475 | 11.379 | 127.250 | 1.00 | 32.58 |
| ATOM | 1209 | N | ARG | A | 155 | 30.443 | 10.999 | 125.035 | 1.00 | 36.63 |
| ATOM | 1210 | CA | ARG | A | 155 | 29.107 | 11.569 | 124.869 | 1.00 | 38.36 |
| ATOM | 1211 | CB | ARG | A | 155 | 28.661 | 11.502 | 123.405 | 1.00 | 36.32 |
| ATOM | 1212 | CG | ARG | A | 155 | 29.581 | 12.253 | 122.460 | 1.00 | 43.15 |
| ATOM | 1213 | CD | ARG | A | 155 | 29.100 | 12.201 | 121.023 | 1.00 | 41.10 |
| ATOM | 1214 | NE | ARG | A | 155 | 27.936 | 13.047 | 120.768 | 1.00 | 44.00 |
| ATOM | 1215 | CZ | ARG | A | 155 | 27.331 | 13.140 | 119.583 | 1.00 | 54.07 |
| ATOM | 1216 | NH1 | ARG | A | 155 | 27.772 | 12.441 | 118.540 | 1.00 | 51.61 |
| ATOM | 1217 | NH2 | ARG | A | 155 | 26.291 | 13.948 | 119.424 | 1.00 | 51.76 |
| ATOM | 1218 | C | ARG | A | 155 | 28.112 | 10.821 | 125.745 | 1.00 | 36.25 |
| ATOM | 1219 | O | ARG | A | 155 | 27.270 | 11.433 | 126.397 | 1.00 | 39.00 |
| ATOM | 1220 | N | LYS | A | 156 | 28.213 | 9.496 | 125.765 | 1.00 | 36.48 |
| ATOM | 1221 | CA | LYS | A | 156 | 27.315 | 8.698 | 126.587 | 1.00 | 39.06 |
| ATOM | 1222 | CB | LYS | A | 156 | 27.460 | 7.213 | 126.256 | 1.00 | 41.88 |
| ATOM | 1223 | CG | LYS | A | 156 | 26.672 | 6.816 | 125.020 | 1.00 | 51.15 |
| ATOM | 1224 | CD | LYS | A | 156 | 27.169 | 7.505 | 123.781 | 1.00 | 55.56 |
| ATOM | 1225 | CE | LYS | A | 156 | 26.117 | 7.502 | 122.676 | 1.00 | 55.63 |
| ATOM | 1226 | NZ | LYS | A | 156 | 24.993 | 8.425 | 123.013 | 1.00 | 49.15 |
| ATOM | 1227 | C | LYS | A | 156 | 27.527 | 8.932 | 128.076 | 1.00 | 39.91 |
| ATOM | 1228 | O | LYS | A | 156 | 26.636 | 8.658 | 128.876 | 1.00 | 37.01 |
| ATOM | 1229 | N | LYS | A | 157 | 28.703 | 9.431 | 128.448 | 1.00 | 37.73 |
| ATOM | 1230 | CA | LYS | A | 157 | 28.985 | 9.725 | 129.847 | 1.00 | 36.52 |
| ATOM | 1231 | CB | LYS | A | 157 | 30.493 | 9.700 | 130.122 | 1.00 | 35.64 |
| ATOM | 1232 | CG | LYS | A | 157 | 31.094 | 8.308 | 130.174 | 1.00 | 35.44 |
| ATOM | 1233 | CD | LYS | A | 157 | 30.509 | 7.510 | 131.335 | 1.00 | 31.28 |
| ATOM | 1234 | CE | LYS | A | 157 | 31.077 | 6.106 | 131.388 | 1.00 | 31.48 |
| ATOM | 1235 | NZ | LYS | A | 157 | 30.464 | 5.310 | 132.493 | 1.00 | 36.39 |
| ATOM | 1236 | C | LYS | A | 157 | 28.423 | 11.097 | 130.197 | 1.00 | 38.12 |
| ATOM | 1237 | O | LYS | A | 157 | 28.531 | 11.547 | 131.336 | 1.00 | 37.61 |
| ATOM | 1238 | N | GLY | A | 158 | 27.842 | 11.768 | 129.205 | 1.00 | 36.27 |
| ATOM | 1239 | CA | GLY | A | 158 | 27.257 | 13.074 | 129.452 | 1.00 | 34.31 |
| ATOM | 1240 | C | GLY | A | 158 | 27.972 | 14.293 | 128.894 | 1.00 | 36.36 |
| ATOM | 1241 | O | GLY | A | 158 | 27.438 | 15.399 | 128.963 | 1.00 | 32.96 |
| ATOM | 1242 | N | PHE | A | 159 | 29.170 | 14.117 | 128.344 | 1.00 | 33.89 |
| ATOM | 1243 | CA | PHE | A | 159 | 29.892 | 15.260 | 127.796 | 1.00 | 30.29 |
| ATOM | 1244 | CB | PHE | A | 159 | 31.346 | 14.892 | 127.504 | 1.00 | 28.62 |
| ATOM | 1245 | CG | PHE | A | 159 | 32.137 | 14.555 | 128.730 | 1.00 | 28.80 |
| ATOM | 1246 | CD1 | PHE | A | 159 | 32.043 | 13.300 | 129.310 | 1.00 | 30.41 |
| ATOM | 1247 | CD2 | PHE | A | 159 | 32.951 | 15.513 | 129.327 | 1.00 | 29.37 |
| ATOM | 1248 | CE1 | PHE | A | 159 | 32.749 | 12.996 | 130.472 | 1.00 | 34.42 |
| ATOM | 1249 | CE2 | PHE | A | 159 | 33.661 | 15.223 | 130.488 | 1.00 | 31.10 |
| ATOM | 1250 | CZ | PHE | A | 159 | 33.561 | 13.963 | 131.062 | 1.00 | 32.32 |
| ATOM | 1251 | C | PHE | A | 159 | 29.224 | 15.786 | 126.536 | 1.00 | 28.88 |
| ATOM | 1252 | O | PHE | A | 159 | 28.765 | 15.003 | 125.705 | 1.00 | 27.71 |
| ATOM | 1253 | N | LYS | A | 160 | 29.180 | 17.110 | 126.402 | 1.00 | 30.20 |
| ATOM | 1254 | CA | LYS | A | 160 | 28.550 | 17.766 | 125.254 | 1.00 | 33.98 |

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Figure 18-20

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1255 | CB | LYS | A | 160 | 27.390 | 18.653 | 125.719 | 1.00 | 36.87 |
| ATOM | 1256 | CG | LYS | A | 160 | 26.273 | 17.914 | 126.419 | 1.00 | 39.48 |
| ATOM | 1257 | CD | LYS | A | 160 | 25.105 | 18.850 | 126.723 | 1.00 | 48.58 |
| ATOM | 1258 | CE | LYS | A | 160 | 25.500 | 20.003 | 127.651 | 1.00 | 50.81 |
| ATOM | 1259 | NZ | LYS | A | 160 | 25.924 | 19.534 | 129.008 | 1.00 | 49.79 |
| ATOM | 1260 | C | LYS | A | 160 | 29.484 | 18.616 | 124.394 | 1.00 | 32.59 |
| ATOM | 1261 | O | LYS | A | 160 | 29.093 | 19.085 | 123.327 | 1.00 | 30.98 |
| ATOM | 1262 | N | ARG | A | 161 | 30.700 | 18.846 | 124.867 | 1.00 | 31.43 |
| ATOM | 1263 | CA | ARG | A | 161 | 31.665 | 19.626 | 124.108 | 1.00 | 29.97 |
| ATOM | 1264 | CB | ARG | A | 161 | 31.781 | 21.048 | 124.673 | 1.00 | 34.45 |
| ATOM | 1265 | CG | ARG | A | 161 | 30.476 | 21.854 | 124.610 | 1.00 | 37.63 |
| ATOM | 1266 | CD | ARG | A | 161 | 30.705 | 23.321 | 124.966 | 1.00 | 39.01 |
| ATOM | 1267 | NE | ARG | A | 161 | 31.158 | 23.503 | 126.341 | 1.00 | 43.76 |
| ATOM | 1268 | CZ | ARG | A | 161 | 30.389 | 23.337 | 127.414 | 1.00 | 43.33 |
| ATOM | 1269 | NH1 | ARG | A | 161 | 29.117 | 22.985 | 127.274 | 1.00 | 45.95 |
| ATOM | 1270 | NH2 | ARG | A | 161 | 30.893 | 23.518 | 128.627 | 1.00 | 43.74 |
| ATOM | 1271 | C | ARG | A | 161 | 33.009 | 18.910 | 124.161 | 1.00 | 32.71 |
| ATOM | 1272 | O | ARG | A | 161 | 33.792 | 19.090 | 125.092 | 1.00 | 28.53 |
| ATOM | 1273 | N | ILE | A | 162 | 33.257 | 18.087 | 123.149 | 1.00 | 32.50 |
| ATOM | 1274 | CA | ILE | A | 162 | 34.485 | 17.313 | 123.049 | 1.00 | 28.52 |
| ATOM | 1275 | CB | ILE | A | 162 | 34.146 | 15.821 | 122.820 | 1.00 | 31.42 |
| ATOM | 1276 | CG2 | ILE | A | 162 | 35.407 | 14.976 | 122.898 | 1.00 | 24.95 |
| ATOM | 1277 | CG1 | ILE | A | 162 | 33.147 | 15.355 | 123.879 | 1.00 | 30.25 |
| ATOM | 1278 | CD1 | ILE | A | 162 | 32.564 | 13.977 | 123.635 | 1.00 | 34.27 |
| ATOM | 1279 | C | ILE | A | 162 | 35.353 | 17.816 | 121.886 | 1.00 | 26.46 |
| ATOM | 1280 | O | ILE | A | 162 | 34.876 | 17.973 | 120.762 | 1.00 | 27.88 |
| ATOM | 1281 | N | LEU | A | 163 | 36.626 | 18.067 | 122.168 | 1.00 | 23.13 |
| ATOM | 1282 | CA | LEU | A | 163 | 37.575 | 18.534 | 121.156 | 1.00 | 25.74 |
| ATOM | 1283 | CB | LEU | A | 163 | 38.384 | 19.729 | 121.681 | 1.00 | 26.25 |
| ATOM | 1284 | CG | LEU | A | 163 | 39.626 | 20.138 | 120.862 | 1.00 | 24.39 |
| ATOM | 1285 | CD1 | LEU | A | 163 | 39.213 | 20.591 | 119.473 | 1.00 | 26.25 |
| ATOM | 1286 | CD2 | LEU | A | 163 | 40.361 | 21.252 | 121.560 | 1.00 | 27.76 |
| ATOM | 1287 | C | LEU | A | 163 | 38.547 | 17.416 | 120.792 | 1.00 | 27.09 |
| ATOM | 1288 | O | LEU | A | 163 | 39.053 | 16.721 | 121.674 | 1.00 | 25.25 |
| ATOM | 1289 | N | TYR | A | 164 | 38.808 | 17.257 | 119.496 | 1.00 | 26.97 |
| ATOM | 1290 | CA | TYR | A | 164 | 39.747 | 16.241 | 119.010 | 1.00 | 26.97 |
| ATOM | 1291 | CB | TYR | A | 164 | 39.021 | 15.181 | 118.179 | 1.00 | 23.38 |
| ATOM | 1292 | CG | TYR | A | 164 | 39.944 | 14.146 | 117.565 | 1.00 | 21.76 |
| ATOM | 1293 | CD1 | TYR | A | 164 | 40.563 | 13.179 | 118.353 | 1.00 | 22.49 |
| ATOM | 1294 | CE1 | TYR | A | 164 | 41.419 | 12.224 | 117.794 | 1.00 | 22.90 |
| ATOM | 1295 | CD2 | TYR | A | 164 | 40.202 | 14.142 | 116.194 | 1.00 | 18.74 |
| ATOM | 1296 | CE2 | TYR | A | 164 | 41.060 | 13.190 | 115.616 | 1.00 | 23.36 |
| ATOM | 1297 | CZ | TYR | A | 164 | 41.663 | 12.235 | 116.426 | 1.00 | 21.50 |
| ATOM | 1298 | OH | TYR | A | 164 | 42.506 | 11.296 | 115.878 | 1.00 | 18.41 |
| ATOM | 1299 | C | TYR | A | 164 | 40.798 | 16.923 | 118.138 | 1.00 | 21.67 |
| ATOM | 1300 | O | TYR | A | 164 | 40.473 | 17.511 | 117.112 | 1.00 | 19.75 |
| ATOM | 1301 | N | ILE | A | 165 | 42.057 | 16.843 | 118.551 | 1.00 | 25.61 |
| ATOM | 1302 | CA | ILE | A | 165 | 43.149 | 17.462 | 117.804 | 1.00 | 24.43 |
| ATOM | 1303 | CB | ILE | A | 165 | 43.963 | 18.396 | 118.717 | 1.00 | 26.41 |
| ATOM | 1304 | CG2 | ILE | A | 165 | 45.127 | 19.017 | 117.937 | 1.00 | 19.36 |
| ATOM | 1305 | CG1 | ILE | A | 165 | 43.035 | 19.482 | 119.274 | 1.00 | 23.36 |
| ATOM | 1306 | CD1 | ILE | A | 165 | 43.685 | 20.402 | 120.299 | 1.00 | 25.05 |
| ATOM | 1307 | C | ILE | A | 165 | 44.040 | 16.365 | 117.234 | 1.00 | 26.91 |
| ATOM | 1308 | O | ILE | A | 165 | 44.538 | 15.505 | 117.971 | 1.00 | 21.91 |
| ATOM | 1309 | N | ASP | A | 166 | 44.242 | 16.408 | 115.920 | 1.00 | 24.20 |
| ATOM | 1310 | CA | ASP | A | 166 | 45.022 | 15.386 | 115.228 | 1.00 | 27.11 |
| ATOM | 1311 | CB | ASP | A | 166 | 44.140 | 14.765 | 114.137 | 1.00 | 28.56 |
| ATOM | 1312 | CG | ASP | A | 166 | 44.699 | 13.461 | 113.599 | 1.00 | 34.59 |
| ATOM | 1313 | OD1 | ASP | A | 166 | 45.831 | 13.456 | 113.068 | 1.00 | 30.37 |
| ATOM | 1314 | OD2 | ASP | A | 166 | 43.995 | 12.437 | 113.717 | 1.00 | 23.27 |
| ATOM | 1315 | C | ASP | A | 166 | 46.319 | 15.924 | 114.614 | 1.00 | 24.47 |
| ATOM | 1316 | O | ASP | A | 166 | 46.295 | 16.613 | 113.591 | 1.00 | 23.19 |
| ATOM | 1317 | N | LEU | A | 167 | 47.452 | 15.597 | 115.227 | 1.00 | 23.43 |
| ATOM | 1318 | CA | LEU | A | 167 | 48.738 | 16.068 | 114.722 | 1.00 | 24.67 |
| ATOM | 1319 | CB | LEU | A | 167 | 49.682 | 16.382 | 115.887 | 1.00 | 21.90 |
| ATOM | 1320 | CG | LEU | A | 167 | 49.143 | 17.444 | 116.858 | 1.00 | 26.62 |

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Figure 18-21

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1321 | CD1 | LEU | A | 167 | 50.249 | 17.845 | 117.821 | 1.00 | 25.88 |
| ATOM | 1322 | CD2 | LEU | A | 167 | 48.658 | 18.668 | 116.092 | 1.00 | 22.40 |
| ATOM | 1323 | C | LEU | A | 167 | 49.405 | 15.092 | 113.755 | 1.00 | 25.82 |
| ATOM | 1324 | O | LEU | A | 167 | 50.504 | 15.345 | 113.262 | 1.00 | 21.89 |
| ATOM | 1325 | N | ASP | A | 168 | 48.736 | 13.977 | 113.488 | 1.00 | 24.69 |
| ATOM | 1326 | CA | ASP | A | 168 | 49.244 | 12.975 | 112.555 | 1.00 | 24.59 |
| ATOM | 1327 | CB | ASP | A | 168 | 48.209 | 11.852 | 112.410 | 1.00 | 27.12 |
| ATOM | 1328 | CG | ASP | A | 168 | 48.722 | 10.669 | 111.608 | 1.00 | 28.11 |
| ATOM | 1329 | C | ASP | A | 168 | 49.423 | 13.686 | 111.209 | 1.00 | 24.17 |
| ATOM | 1330 | O | ASP | A | 168 | 48.629 | 14.559 | 110.865 | 1.00 | 17.18 |
| ATOM | 1331 | OD1 | ASP | A | 168 | 49.085 | 9.644 | 112.227 | 1.00 | 25.40 |
| ATOM | 1332 | OD2 | ASP | A | 168 | 48.777 | 10.750 | 110.364 | 1.00 | 34.72 |
| ATOM | 1333 | N | ALA | A | 169 | 50.448 | 13.312 | 110.446 | 1.00 | 21.29 |
| ATOM | 1334 | CA | ALA | A | 169 | 50.693 | 13.927 | 109.140 | 1.00 | 25.00 |
| ATOM | 1335 | CB | ALA | A | 169 | 52.068 | 13.498 | 108.601 | 1.00 | 21.17 |
| ATOM | 1336 | C | ALA | A | 169 | 49.612 | 13.636 | 108.093 | 1.00 | 26.57 |
| ATOM | 1337 | O | ALA | A | 169 | 49.641 | 14.204 | 107.000 | 1.00 | 26.90 |
| ATOM | 1338 | N | HIS | A | 170 | 48.673 | 12.746 | 108.406 | 1.00 | 21.63 |
| ATOM | 1339 | CA | HIS | A | 170 | 47.592 | 12.445 | 107.468 | 1.00 | 24.79 |
| ATOM | 1340 | C | HIS | A | 170 | 46.243 | 12.867 | 108.045 | 1.00 | 20.98 |
| ATOM | 1341 | O | HIS | A | 170 | 46.044 | 12.849 | 109.255 | 1.00 | 24.12 |
| ATOM | 1342 | CB | HIS | A | 170 | 47.550 | 10.950 | 107.131 | 1.00 | 23.17 |
| ATOM | 1343 | CG | HIS | A | 170 | 48.830 | 10.420 | 106.570 | 1.00 | 30.28 |
| ATOM | 1344 | ND1 | HIS | A | 170 | 49.842 | 9.982 | 107.385 | 1.00 | 31.00 |
| ATOM | 1345 | CE1 | HIS | A | 170 | 50.825 | 9.634 | 106.577 | 1.00 | 24.33 |
| ATOM | 1346 | CD2 | HIS | A | 170 | 49.224 | 10.329 | 105.273 | 1.00 | 22.88 |
| ATOM | 1347 | NE2 | HIS | A | 170 | 50.502 | 9.828 | 105.285 | 1.00 | 21.89 |
| ATOM | 1348 | N | HIS | A | 171 | 45.317 | 13.231 | 107.171 | 1.00 | 21.14 |
| ATOM | 1349 | CA | HIS | A | 171 | 43.993 | 13.661 | 107.591 | 1.00 | 25.57 |
| ATOM | 1350 | CB | HIS | A | 171 | 43.234 | 14.242 | 106.404 | 1.00 | 22.47 |
| ATOM | 1351 | CG | HIS | A | 171 | 41.857 | 14.719 | 106.746 | 1.00 | 29.75 |
| ATOM | 1352 | CD2 | HIS | A | 171 | 41.433 | 15.648 | 107.634 | 1.00 | 25.58 |
| ATOM | 1353 | ND1 | HIS | A | 171 | 40.721 | 14.201 | 106.160 | 1.00 | 28.90 |
| ATOM | 1354 | CE1 | HIS | A | 171 | 39.656 | 14.787 | 106.676 | 1.00 | 25.35 |
| ATOM | 1355 | NE2 | HIS | A | 171 | 40.060 | 15.669 | 107.573 | 1.00 | 32.40 |
| ATOM | 1356 | C | HIS | A | 171 | 43.169 | 12.533 | 108.204 | 1.00 | 29.61 |
| ATOM | 1357 | O | HIS | A | 171 | 43.169 | 11.411 | 107.698 | 1.00 | 27.62 |
| ATOM | 1358 | N | CYS | A | 172 | 42.461 | 12.852 | 109.286 | 1.00 | 26.52 |
| ATOM | 1359 | CA | CYS | A | 172 | 41.610 | 11.897 | 109.987 | 1.00 | 24.82 |
| ATOM | 1360 | CB | CYS | A | 172 | 41.460 | 12.322 | 111.456 | 1.00 | 29.47 |
| ATOM | 1361 | SG | CYS | A | 172 | 40.959 | 14.065 | 111.717 | 1.00 | 25.69 |
| ATOM | 1362 | C | CYS | A | 172 | 40.237 | 11.797 | 109.314 | 1.00 | 28.21 |
| ATOM | 1363 | O | CYS | A | 172 | 39.211 | 12.131 | 109.914 | 1.00 | 26.78 |
| ATOM | 1364 | N | ASP | A | 173 | 40.213 | 11.332 | 108.066 | 1.00 | 22.05 |
| ATOM | 1365 | CA | ASP | A | 173 | 38.949 | 11.217 | 107.350 | 1.00 | 27.39 |
| ATOM | 1366 | CB | ASP | A | 173 | 39.167 | 10.646 | 105.931 | 1.00 | 30.47 |
| ATOM | 1367 | CG | ASP | A | 173 | 39.824 | 9.264 | 105.922 | 1.00 | 29.77 |
| ATOM | 1368 | OD1 | ASP | A | 173 | 39.886 | 8.658 | 104.830 | 1.00 | 21.14 |
| ATOM | 1369 | OD2 | ASP | A | 173 | 40.288 | 8.787 | 106.978 | 1.00 | 30.04 |
| ATOM | 1370 | C | ASP | A | 173 | 37.895 | 10.400 | 108.105 | 1.00 | 27.86 |
| ATOM | 1371 | O | ASP | A | 173 | 36.720 | 10.762 | 108.120 | 1.00 | 23.47 |
| ATOM | 1372 | N | GLY | A | 174 | 38.309 | 9.315 | 108.753 | 1.00 | 25.84 |
| ATOM | 1373 | CA | GLY | A | 174 | 37.344 | 8.513 | 109.490 | 1.00 | 28.49 |
| ATOM | 1374 | C | GLY | A | 174 | 36.694 | 9.296 | 110.619 | 1.00 | 26.14 |
| ATOM | 1375 | O | GLY | A | 174 | 35.475 | 9.287 | 110.780 | 1.00 | 21.39 |
| ATOM | 1376 | N | VAL | A | 175 | 37.510 | 9.984 | 111.409 | 1.00 | 27.24 |
| ATOM | 1377 | CA | VAL | A | 175 | 36.995 | 10.773 | 112.523 | 1.00 | 25.53 |
| ATOM | 1378 | CB | VAL | A | 175 | 38.137 | 11.299 | 113.401 | 1.00 | 30.54 |
| ATOM | 1379 | CG1 | VAL | A | 175 | 37.565 | 12.105 | 114.566 | 1.00 | 28.02 |
| ATOM | 1380 | CG2 | VAL | A | 175 | 38.973 | 10.129 | 113.911 | 1.00 | 21.30 |
| ATOM | 1381 | C | VAL | A | 175 | 36.163 | 11.955 | 112.035 | 1.00 | 25.01 |
| ATOM | 1382 | O | VAL | A | 175 | 35.130 | 12.282 | 112.623 | 1.00 | 21.60 |
| ATOM | 1383 | N | GLN | A | 176 | 36.601 | 12.594 | 110.957 | 1.00 | 25.43 |
| ATOM | 1384 | CA | GLN | A | 176 | 35.854 | 13.730 | 110.426 | 1.00 | 26.12 |
| ATOM | 1385 | CB | GLN | A | 176 | 36.554 | 14.336 | 109.205 | 1.00 | 24.71 |
| ATOM | 1386 | CG | GLN | A | 176 | 35.682 | 15.349 | 108.469 | 1.00 | 26.68 |

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Figure 18-22

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1387 | CD | GLN | A | 176 | 36.385 | 16.002 | 107.306 | 1.00 | 29.54 |
| ATOM | 1388 | OE1 | GLN | A | 176 | 37.382 | 16.704 | 107.486 | 1.00 | 26.93 |
| ATOM | 1389 | NE2 | GLN | A | 176 | 35.872 | 15.776 | 106.099 | 1.00 | 27.58 |
| ATOM | 1390 | C | GLN | A | 176 | 34.446 | 13.316 | 110.029 | 1.00 | 27.63 |
| ATOM | 1391 | O | GLN | A | 176 | 33.481 | 14.021 | 110.319 | 1.00 | 25.93 |
| ATOM | 1392 | N | GLU | A | 177 | 34.330 | 12.173 | 109.362 | 1.00 | 32.21 |
| ATOM | 1393 | CA | GLU | A | 177 | 33.027 | 11.696 | 108.915 | 1.00 | 32.72 |
| ATOM | 1394 | CB | GLU | A | 177 | 33.181 | 10.445 | 108.053 | 1.00 | 34.20 |
| ATOM | 1395 | CG | GLU | A | 177 | 31.905 | 10.069 | 107.329 | 1.00 | 39.40 |
| ATOM | 1396 | CD | GLU | A | 177 | 32.060 | 8.819 | 106.497 | 1.00 | 41.42 |
| ATOM | 1397 | OE1 | GLU | A | 177 | 32.056 | 7.712 | 107.075 | 1.00 | 45.91 |
| ATOM | 1398 | OE2 | GLU | A | 177 | 32.206 | 8.947 | 105.264 | 1.00 | 42.35 |
| ATOM | 1399 | C | GLU | A | 177 | 32.128 | 11.377 | 110.099 | 1.00 | 30.54 |
| ATOM | 1400 | O | GLU | A | 177 | 30.945 | 11.697 | 110.093 | 1.00 | 25.39 |
| ATOM | 1401 | N | ALA | A | 178 | 32.707 | 10.750 | 111.114 | 1.00 | 27.03 |
| ATOM | 1402 | CA | ALA | A | 178 | 31.971 | 10.365 | 112.303 | 1.00 | 30.67 |
| ATOM | 1403 | CB | ALA | A | 178 | 32.905 | 9.658 | 113.289 | 1.00 | 30.49 |
| ATOM | 1404 | C | ALA | A | 178 | 31.261 | 11.519 | 113.003 | 1.00 | 33.21 |
| ATOM | 1405 | O | ALA | A | 178 | 30.145 | 11.355 | 113.493 | 1.00 | 28.64 |
| ATOM | 1406 | N | PHE | A | 179 | 31.888 | 12.688 | 113.055 | 1.00 | 29.27 |
| ATOM | 1407 | CA | PHE | A | 179 | 31.256 | 13.801 | 113.751 | 1.00 | 30.49 |
| ATOM | 1408 | CB | PHE | A | 179 | 32.071 | 14.128 | 115.001 | 1.00 | 24.44 |
| ATOM | 1409 | CG | PHE | A | 179 | 32.469 | 12.909 | 115.781 | 1.00 | 24.43 |
| ATOM | 1410 | CD1 | PHE | A | 179 | 33.749 | 12.375 | 115.657 | 1.00 | 25.04 |
| ATOM | 1411 | CD2 | PHE | A | 179 | 31.536 | 12.233 | 116.563 | 1.00 | 23.09 |
| ATOM | 1412 | CE1 | PHE | A | 179 | 34.103 | 11.184 | 116.293 | 1.00 | 16.56 |
| ATOM | 1413 | CE2 | PHE | A | 179 | 31.881 | 11.038 | 117.204 | 1.00 | 26.38 |
| ATOM | 1414 | CZ | PHE | A | 179 | 33.170 | 10.515 | 117.067 | 1.00 | 20.30 |
| ATOM | 1415 | C | PHE | A | 179 | 31.079 | 15.037 | 112.891 | 1.00 | 31.00 |
| ATOM | 1416 | O | PHE | A | 179 | 31.006 | 16.152 | 113.399 | 1.00 | 31.32 |
| ATOM | 1417 | N | TYR | A | 180 | 30.980 | 14.828 | 111.584 | 1.00 | 31.68 |
| ATOM | 1418 | CA | TYR | A | 180 | 30.829 | 15.925 | 110.646 | 1.00 | 32.76 |
| ATOM | 1419 | CB | TYR | A | 180 | 30.931 | 15.378 | 109.213 | 1.00 | 35.12 |
| ATOM | 1420 | CG | TYR | A | 180 | 31.331 | 16.406 | 108.172 | 1.00 | 36.27 |
| ATOM | 1421 | CD1 | TYR | A | 180 | 30.427 | 16.846 | 107.204 | 1.00 | 37.31 |
| ATOM | 1422 | CE1 | TYR | A | 180 | 30.801 | 17.791 | 106.244 | 1.00 | 34.81 |
| ATOM | 1423 | CD2 | TYR | A | 180 | 32.624 | 16.937 | 108.154 | 1.00 | 36.32 |
| ATOM | 1424 | CE2 | TYR | A | 180 | 33.007 | 17.879 | 107.203 | 1.00 | 37.83 |
| ATOM | 1425 | CZ | TYR | A | 180 | 32.088 | 18.304 | 106.250 | 1.00 | 36.05 |
| ATOM | 1426 | OH | TYR | A | 180 | 32.446 | 19.255 | 105.323 | 1.00 | 28.04 |
| ATOM | 1427 | C | TYR | A | 180 | 29.518 | 16.696 | 110.825 | 1.00 | 30.94 |
| ATOM | 1428 | O | TYR | A | 180 | 29.459 | 17.894 | 110.560 | 1.00 | 30.42 |
| ATOM | 1429 | N | ASP | A | 181 | 28.473 | 16.026 | 111.299 | 1.00 | 31.56 |
| ATOM | 1430 | CA | ASP | A | 181 | 27.180 | 16.691 | 111.444 | 1.00 | 37.30 |
| ATOM | 1431 | CB | ASP | A | 181 | 26.086 | 15.833 | 110.807 | 1.00 | 37.68 |
| ATOM | 1432 | CG | ASP | A | 181 | 25.645 | 14.689 | 111.705 | 1.00 | 39.86 |
| ATOM | 1433 | OD1 | ASP | A | 181 | 26.505 | 13.963 | 112.233 | 1.00 | 43.25 |
| ATOM | 1434 | OD2 | ASP | A | 181 | 24.425 | 14.504 | 111.871 | 1.00 | 46.56 |
| ATOM | 1435 | C | ASP | A | 181 | 26.754 | 17.044 | 112.866 | 1.00 | 36.81 |
| ATOM | 1436 | O | ASP | A | 181 | 25.571 | 17.286 | 113.109 | 1.00 | 33.91 |
| ATOM | 1437 | N | THR | A | 182 | 27.689 | 17.066 | 113.810 | 1.00 | 40.86 |
| ATOM | 1438 | CA | THR | A | 182 | 27.327 | 17.412 | 115.184 | 1.00 | 38.27 |
| ATOM | 1439 | CB | THR | A | 182 | 27.433 | 16.201 | 116.133 | 1.00 | 37.99 |
| ATOM | 1440 | OG1 | THR | A | 182 | 27.013 | 16.595 | 117.448 | 1.00 | 35.64 |
| ATOM | 1441 | CG2 | THR | A | 182 | 28.869 | 15.684 | 116.194 | 1.00 | 35.61 |
| ATOM | 1442 | C | THR | A | 182 | 28.177 | 18.546 | 115.746 | 1.00 | 39.51 |
| ATOM | 1443 | O | THR | A | 182 | 29.365 | 18.673 | 115.433 | 1.00 | 40.07 |
| ATOM | 1444 | N | ASP | A | 183 | 27.557 | 19.369 | 116.582 | 1.00 | 37.01 |
| ATOM | 1445 | CA | ASP | A | 183 | 28.250 | 20.497 | 117.181 | 1.00 | 37.74 |
| ATOM | 1446 | CB | ASP | A | 183 | 27.313 | 21.706 | 117.228 | 1.00 | 35.56 |
| ATOM | 1447 | CG | ASP | A | 183 | 26.136 | 21.493 | 118.155 | 1.00 | 38.01 |
| ATOM | 1448 | OD1 | ASP | A | 183 | 25.614 | 20.357 | 118.210 | 1.00 | 34.94 |
| ATOM | 1449 | OD2 | ASP | A | 183 | 25.720 | 22.470 | 118.814 | 1.00 | 38.17 |
| ATOM | 1450 | C | ASP | A | 183 | 28.762 | 20.161 | 118.578 | 1.00 | 35.27 |
| ATOM | 1451 | O | ASP | A | 183 | 29.337 | 21.015 | 119.251 | 1.00 | 35.16 |
| ATOM | 1452 | N | GLN | A | 184 | 28.562 | 18.917 | 119.012 | 1.00 | 35.10 |

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Figure 18-23

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 1453 | CA | GLN A 184 | 29.030 | 18.505 | 120.333 | 1.00 | 35.16 |
| ATOM | 1454 | CB | GLN A 184 | 28.155 | 17.382 | 120.906 | 1.00 | 36.94 |
| ATOM | 1455 | CG | GLN A 184 | 26.663 | 17.718 | 120.988 | 1.00 | 38.34 |
| ATOM | 1456 | CD | GLN A 184 | 25.881 | 16.725 | 121.838 | 1.00 | 43.68 |
| ATOM | 1457 | OE1 | GLN A 184 | 26.027 | 15.512 | 121.696 | 1.00 | 35.48 |
| ATOM | 1458 | NE2 | GLN A 184 | 25.036 | 17.243 | 122.723 | 1.00 | 51.06 |
| ATOM | 1459 | C | GLN A 184 | 30.479 | 18.035 | 120.253 | 1.00 | 36.32 |
| ATOM | 1460 | O | GLN A 184 | 31.135 | 17.825 | 121.275 | 1.00 | 34.24 |
| ATOM | 1461 | N | VAL A 185 | 30.976 | 17.883 | 119.028 | 1.00 | 34.51 |
| ATOM | 1462 | CA | VAL A 185 | 32.348 | 17.443 | 118.804 | 1.00 | 33.59 |
| ATOM | 1463 | CB | VAL A 185 | 32.393 | 15.990 | 118.259 | 1.00 | 35.11 |
| ATOM | 1464 | CG1 | VAL A 185 | 33.834 | 15.567 | 118.003 | 1.00 | 23.80 |
| ATOM | 1465 | CG2 | VAL A 185 | 31.731 | 15.045 | 119.242 | 1.00 | 26.00 |
| ATOM | 1466 | C | VAL A 185 | 33.053 | 18.354 | 117.803 | 1.00 | 33.11 |
| ATOM | 1467 | O | VAL A 185 | 32.545 | 18.593 | 116.714 | 1.00 | 27.73 |
| ATOM | 1468 | N | PHE A 186 | 34.215 | 18.872 | 118.184 | 1.00 | 31.49 |
| ATOM | 1469 | CA | PHE A 186 | 34.985 | 19.729 | 117.291 | 1.00 | 30.63 |
| ATOM | 1470 | CB | PHE A 186 | 35.420 | 21.023 | 117.991 | 1.00 | 30.34 |
| ATOM | 1471 | CG | PHE A 186 | 36.008 | 22.047 | 117.051 | 1.00 | 30.22 |
| ATOM | 1472 | CD1 | PHE A 186 | 35.265 | 23.156 | 116.656 | 1.00 | 32.23 |
| ATOM | 1473 | CD2 | PHE A 186 | 37.284 | 21.879 | 116.524 | 1.00 | 29.37 |
| ATOM | 1474 | CE1 | PHE A 186 | 35.785 | 24.078 | 115.748 | 1.00 | 27.87 |
| ATOM | 1475 | CE2 | PHE A 186 | 37.813 | 22.794 | 115.615 | 1.00 | 28.54 |
| ATOM | 1476 | CZ | PHE A 186 | 37.064 | 23.892 | 115.227 | 1.00 | 30.80 |
| ATOM | 1477 | C | PHE A 186 | 36.232 | 18.952 | 116.879 | 1.00 | 33.38 |
| ATOM | 1478 | O | PHE A 186 | 36.952 | 18.426 | 117.729 | 1.00 | 28.30 |
| ATOM | 1479 | N | VAL A 187 | 36.478 | 18.877 | 115.574 | 1.00 | 32.00 |
| ATOM | 1480 | CA | VAL A 187 | 37.645 | 18.171 | 115.060 | 1.00 | 29.70 |
| ATOM | 1481 | CB | VAL A 187 | 37.252 | 17.095 | 114.019 | 1.00 | 30.03 |
| ATOM | 1482 | CG1 | VAL A 187 | 38.510 | 16.488 | 113.405 | 1.00 | 27.77 |
| ATOM | 1483 | CG2 | VAL A 187 | 36.410 | 16.003 | 114.672 | 1.00 | 25.98 |
| ATOM | 1484 | C | VAL A 187 | 38.604 | 19.153 | 114.392 | 1.00 | 31.03 |
| ATOM | 1485 | O | VAL A 187 | 38.215 | 19.895 | 113.491 | 1.00 | 31.88 |
| ATOM | 1486 | N | LEU A 188 | 39.850 | 19.157 | 114.857 | 1.00 | 24.88 |
| ATOM | 1487 | CA | LEU A 188 | 40.899 | 20.010 | 114.304 | 1.00 | 26.92 |
| ATOM | 1488 | CB | LEU A 188 | 41.468 | 20.959 | 115.361 | 1.00 | 27.04 |
| ATOM | 1489 | CG | LEU A 188 | 42.823 | 21.565 | 114.963 | 1.00 | 25.15 |
| ATOM | 1490 | CD1 | LEU A 188 | 42.686 | 22.315 | 113.648 | 1.00 | 18.53 |
| ATOM | 1491 | CD2 | LEU A 188 | 43.330 | 22.485 | 116.068 | 1.00 | 28.81 |
| ATOM | 1492 | C | LEU A 188 | 42.022 | 19.113 | 113.815 | 1.00 | 31.22 |
| ATOM | 1493 | O | LEU A 188 | 42.579 | 18.333 | 114.587 | 1.00 | 25.83 |
| ATOM | 1494 | N | SER A 189 | 42.369 | 19.230 | 112.540 | 1.00 | 30.53 |
| ATOM | 1495 | CA | SER A 189 | 43.429 | 18.399 | 112.007 | 1.00 | 30.13 |
| ATOM | 1496 | CB | SER A 189 | 42.821 | 17.249 | 111.199 | 1.00 | 33.41 |
| ATOM | 1497 | OG | SER A 189 | 43.837 | 16.474 | 110.588 | 1.00 | 32.98 |
| ATOM | 1498 | C | SER A 189 | 44.448 | 19.120 | 111.143 | 1.00 | 27.94 |
| ATOM | 1499 | O | SER A 189 | 44.084 | 19.891 | 111.253 | 1.00 | 22.14 |
| ATOM | 1500 | N | LEU A 190 | 45.728 | 18.877 | 111.423 | 1.00 | 24.80 |
| ATOM | 1501 | CA | LEU A 190 | 46.805 | 19.438 | 110.614 | 1.00 | 22.23 |
| ATOM | 1502 | CB | LEU A 190 | 47.955 | 20.000 | 111.459 | 1.00 | 23.69 |
| ATOM | 1503 | CG | LEU A 190 | 47.733 | 21.075 | 112.522 | 1.00 | 28.92 |
| ATOM | 1504 | CD1 | LEU A 190 | 49.070 | 21.780 | 112.740 | 1.00 | 23.01 |
| ATOM | 1505 | CD2 | LEU A 190 | 46.691 | 22.093 | 112.087 | 1.00 | 28.11 |
| ATOM | 1506 | C | LEU A 190 | 47.300 | 18.210 | 109.872 | 1.00 | 22.69 |
| ATOM | 1507 | O | LEU A 190 | 47.416 | 17.141 | 110.465 | 1.00 | 16.55 |
| ATOM | 1508 | N | HIS A 191 | 47.599 | 18.353 | 108.587 | 1.00 | 19.22 |
| ATOM | 1509 | CA | HIS A 191 | 48.046 | 17.210 | 107.804 | 1.00 | 23.28 |
| ATOM | 1510 | CB | HIS A 191 | 46.870 | 16.242 | 107.650 | 1.00 | 15.58 |
| ATOM | 1511 | CG | HIS A 191 | 45.591 | 16.915 | 107.256 | 1.00 | 24.16 |
| ATOM | 1512 | CD2 | HIS A 191 | 45.034 | 17.124 | 106.038 | 1.00 | 17.71 |
| ATOM | 1513 | ND1 | HIS A 191 | 44.695 | 17.419 | 108.176 | 1.00 | 23.76 |
| ATOM | 1514 | CE1 | HIS A 191 | 43.644 | 17.913 | 107.545 | 1.00 | 19.78 |
| ATOM | 1515 | NE2 | HIS A 191 | 43.823 | 17.746 | 106.246 | 1.00 | 27.87 |
| ATOM | 1516 | C | HIS A 191 | 48.570 | 17.620 | 106.434 | 1.00 | 23.65 |
| ATOM | 1517 | O | HIS A 191 | 48.419 | 18.761 | 106.017 | 1.00 | 23.89 |
| ATOM | 1518 | N | GLN A 192 | 49.209 | 16.681 | 105.746 | 1.00 | 23.49 |

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Figure 18-24

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1519 | CA | GLN | A | 192 | 49.718 | 16.950 | 104.412 | 1.00 | 20.55 |
| ATOM | 1520 | CB | GLN | A | 192 | 50.474 | 15.738 | 103.864 | 1.00 | 23.63 |
| ATOM | 1521 | CG | GLN | A | 192 | 51.528 | 15.181 | 104.797 | 1.00 | 24.07 |
| ATOM | 1522 | CD | GLN | A | 192 | 52.110 | 13.876 | 104.293 | 1.00 | 26.90 |
| ATOM | 1523 | OE1 | GLN | A | 192 | 52.986 | 13.860 | 103.421 | 1.00 | 20.21 |
| ATOM | 1524 | NE2 | GLN | A | 192 | 51.605 | 12.765 | 104.828 | 1.00 | 23.52 |
| ATOM | 1525 | C | GLN | A | 192 | 48.478 | 17.174 | 103.570 | 1.00 | 21.41 |
| ATOM | 1526 | O | GLN | A | 192 | 47.478 | 16.466 | 103.726 | 1.00 | 20.15 |
| ATOM | 1527 | N | SER | A | 193 | 48.528 | 18.167 | 102.692 | 1.00 | 24.36 |
| ATOM | 1528 | CA | SER | A | 193 | 47.397 | 18.448 | 101.821 | 1.00 | 23.98 |
| ATOM | 1529 | CB | SER | A | 193 | 47.760 | 19.537 | 100.820 | 1.00 | 24.60 |
| ATOM | 1530 | OG | SER | A | 193 | 46.729 | 19.660 | 99.861 | 1.00 | 25.83 |
| ATOM | 1531 | C | SER | A | 193 | 46.985 | 17.200 | 101.045 | 1.00 | 23.74 |
| ATOM | 1532 | O | SER | A | 193 | 47.829 | 16.492 | 100.506 | 1.00 | 19.80 |
| ATOM | 1533 | N | PRO | A | 194 | 45.674 | 16.936 | 100.953 | 1.00 | 24.85 |
| ATOM | 1534 | CD | PRO | A | 194 | 44.561 | 17.719 | 101.507 | 1.00 | 25.08 |
| ATOM | 1535 | CA | PRO | A | 194 | 45.151 | 15.772 | 100.235 | 1.00 | 29.25 |
| ATOM | 1536 | CB | PRO | A | 194 | 43.641 | 15.901 | 100.444 | 1.00 | 30.51 |
| ATOM | 1537 | CG | PRO | A | 194 | 43.554 | 16.643 | 101.758 | 1.00 | 30.21 |
| ATOM | 1538 | C | PRO | A | 194 | 45.527 | 15.825 | 98.756 | 1.00 | 30.75 |
| ATOM | 1539 | O | PRO | A | 194 | 45.420 | 14.830 | 98.041 | 1.00 | 30.04 |
| ATOM | 1540 | N | GLU | A | 195 | 45.967 | 16.991 | 98.298 | 1.00 | 26.28 |
| ATOM | 1541 | CA | GLU | A | 195 | 46.343 | 17.127 | 96.898 | 1.00 | 31.11 |
| ATOM | 1542 | CB | GLU | A | 195 | 46.738 | 18.570 | 96.571 | 1.00 | 29.52 |
| ATOM | 1543 | CG | GLU | A | 195 | 45.680 | 19.600 | 96.933 | 1.00 | 38.32 |
| ATOM | 1544 | CD | GLU | A | 195 | 45.976 | 20.972 | 96.352 | 1.00 | 44.15 |
| ATOM | 1545 | OE1 | GLU | A | 195 | 47.139 | 21.425 | 96.434 | 1.00 | 44.23 |
| ATOM | 1546 | OE2 | GLU | A | 195 | 45.037 | 21.605 | 95.825 | 1.00 | 45.06 |
| ATOM | 1547 | C | GLU | A | 195 | 47.499 | 16.193 | 96.552 | 1.00 | 30.81 |
| ATOM | 1548 | O | GLU | A | 195 | 47.582 | 15.705 | 95.426 | 1.00 | 37.17 |
| ATOM | 1549 | N | TYR | A | 196 | 48.377 | 15.922 | 97.515 | 1.00 | 25.01 |
| ATOM | 1550 | CA | TYR | A | 196 | 49.517 | 15.053 | 97.242 | 1.00 | 23.43 |
| ATOM | 1551 | CB | TYR | A | 196 | 50.810 | 15.881 | 97.223 | 1.00 | 26.67 |
| ATOM | 1552 | CG | TYR | A | 196 | 51.255 | 16.424 | 98.572 | 1.00 | 26.78 |
| ATOM | 1553 | CD1 | TYR | A | 196 | 51.957 | 15.625 | 99.476 | 1.00 | 26.08 |
| ATOM | 1554 | CE1 | TYR | A | 196 | 52.338 | 16.110 | 100.734 | 1.00 | 26.77 |
| ATOM | 1555 | CD2 | TYR | A | 196 | 50.944 | 17.731 | 98.958 | 1.00 | 27.55 |
| ATOM | 1556 | CE2 | TYR | A | 196 | 51.320 | 18.226 | 100.216 | 1.00 | 25.95 |
| ATOM | 1557 | CZ | TYR | A | 196 | 52.012 | 17.409 | 101.096 | 1.00 | 24.78 |
| ATOM | 1558 | OH | TYR | A | 196 | 52.356 | 17.879 | 102.345 | 1.00 | 25.50 |
| ATOM | 1559 | C | TYR | A | 196 | 49.670 | 13.906 | 98.229 | 1.00 | 27.05 |
| ATOM | 1560 | O | TYR | A | 196 | 50.585 | 13.088 | 98.096 | 1.00 | 24.02 |
| ATOM | 1561 | N | ALA | A | 197 | 48.785 | 13.822 | 99.214 | 1.00 | 22.10 |
| ATOM | 1562 | CA | ALA | A | 197 | 48.928 | 12.760 | 100.199 | 1.00 | 24.90 |
| ATOM | 1563 | CB | ALA | A | 197 | 49.627 | 13.307 | 101.437 | 1.00 | 27.83 |
| ATOM | 1564 | C | ALA | A | 197 | 47.644 | 12.069 | 100.608 | 1.00 | 26.20 |
| ATOM | 1565 | O | ALA | A | 197 | 46.553 | 12.617 | 100.484 | 1.00 | 22.82 |
| ATOM | 1566 | N | PHE | A | 198 | 47.795 | 10.849 | 101.102 | 1.00 | 31.74 |
| ATOM | 1567 | CA | PHE | A | 198 | 46.663 | 10.072 | 101.580 | 1.00 | 28.74 |
| ATOM | 1568 | CB | PHE | A | 198 | 47.130 | 8.691 | 102.036 | 1.00 | 30.66 |
| ATOM | 1569 | CG | PHE | A | 198 | 46.009 | 7.766 | 102.399 | 1.00 | 29.61 |
| ATOM | 1570 | CD1 | PHE | A | 198 | 45.496 | 6.879 | 101.463 | 1.00 | 28.76 |
| ATOM | 1571 | CD2 | PHE | A | 198 | 45.426 | 7.822 | 103.657 | 1.00 | 28.43 |
| ATOM | 1572 | CE1 | PHE | A | 198 | 44.415 | 6.057 | 101.773 | 1.00 | 35.72 |
| ATOM | 1573 | CE2 | PHE | A | 198 | 44.340 | 7.004 | 103.970 | 1.00 | 34.62 |
| ATOM | 1574 | CZ | PHE | A | 198 | 43.837 | 6.121 | 103.029 | 1.00 | 35.73 |
| ATOM | 1575 | C | PHE | A | 198 | 46.121 | 10.814 | 102.802 | 1.00 | 28.95 |
| ATOM | 1576 | O | PHE | A | 198 | 46.892 | 11.347 | 103.596 | 1.00 | 25.72 |
| ATOM | 1577 | N | PRO | A | 199 | 44.792 | 10.905 | 102.941 | 1.00 | 28.27 |
| ATOM | 1578 | CD | PRO | A | 199 | 44.100 | 11.499 | 104.099 | 1.00 | 33.97 |
| ATOM | 1579 | CA | PRO | A | 199 | 43.813 | 10.364 | 102.008 | 1.00 | 32.80 |
| ATOM | 1580 | CB | PRO | A | 199 | 42.550 | 10.312 | 102.858 | 1.00 | 29.84 |
| ATOM | 1581 | CG | PRO | A | 199 | 42.665 | 11.612 | 103.592 | 1.00 | 37.32 |
| ATOM | 1582 | C | PRO | A | 199 | 43.773 | 11.476 | 100.965 | 1.00 | 35.02 |
| ATOM | 1583 | O | PRO | A | 199 | 44.052 | 12.631 | 101.280 | 1.00 | 48.84 |
| ATOM | 1584 | N | PHE | A | 200 | 43.441 | 11.156 | 99.734 | 1.00 | 33.64 |

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Figure 18-25

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1585 | CA | PHE | A | 200 | 43.418 | 12.179 | 98.718 | 1.00 | 28.12 |
| ATOM | 1586 | CB | PHE | A | 200 | 43.927 | 11.579 | 97.411 | 1.00 | 26.69 |
| ATOM | 1587 | CG | PHE | A | 200 | 45.226 | 10.833 | 97.561 | 1.00 | 27.33 |
| ATOM | 1588 | CD1 | PHE | A | 200 | 45.239 | 9.510 | 97.995 | 1.00 | 29.79 |
| ATOM | 1589 | CD2 | PHE | A | 200 | 46.439 | 11.461 | 97.302 | 1.00 | 24.38 |
| ATOM | 1590 | CE1 | PHE | A | 200 | 46.444 | 8.820 | 98.168 | 1.00 | 29.45 |
| ATOM | 1591 | CE2 | PHE | A | 200 | 47.651 | 10.782 | 97.473 | 1.00 | 31.41 |
| ATOM | 1592 | CZ | PHE | A | 200 | 47.653 | 9.458 | 97.906 | 1.00 | 29.64 |
| ATOM | 1593 | C | PHE | A | 200 | 42.042 | 12.795 | 98.518 | 1.00 | 26.15 |
| ATOM | 1594 | O | PHE | A | 200 | 41.935 | 13.889 | 97.986 | 1.00 | 27.96 |
| ATOM | 1595 | N | GLU | A | 201 | 41.002 | 12.101 | 98.979 | 1.00 | 28.52 |
| ATOM | 1596 | CA | GLU | A | 201 | 39.614 | 12.534 | 98.806 | 1.00 | 35.04 |
| ATOM | 1597 | CB | GLU | A | 201 | 38.695 | 11.316 | 98.819 | 1.00 | 33.61 |
| ATOM | 1598 | CG | GLU | A | 201 | 39.087 | 10.240 | 97.838 | 1.00 | 37.80 |
| ATOM | 1599 | CD | GLU | A | 201 | 38.222 | 9.016 | 97.997 | 1.00 | 43.48 |
| ATOM | 1600 | OE1 | GLU | A | 201 | 36.992 | 9.142 | 97.825 | 1.00 | 40.96 |
| ATOM | 1601 | OE2 | GLU | A | 201 | 38.772 | 7.937 | 98.298 | 1.00 | 44.17 |
| ATOM | 1602 | C | GLU | A | 201 | 39.077 | 13.516 | 99.837 | 1.00 | 36.30 |
| ATOM | 1603 | O | GLU | A | 201 | 38.087 | 14.206 | 99.592 | 1.00 | 36.47 |
| ATOM | 1604 | N | LYS | A | 202 | 39.693 | 13.552 | 101.007 | 1.00 | 34.63 |
| ATOM | 1605 | CA | LYS | A | 202 | 39.229 | 14.460 | 102.030 | 1.00 | 34.09 |
| ATOM | 1606 | CB | LYS | A | 202 | 38.294 | 13.729 | 102.992 | 1.00 | 40.88 |
| ATOM | 1607 | CG | LYS | A | 202 | 37.011 | 13.318 | 102.292 | 1.00 | 43.17 |
| ATOM | 1608 | CD | LYS | A | 202 | 35.935 | 12.854 | 103.230 | 1.00 | 47.39 |
| ATOM | 1609 | CE | LYS | A | 202 | 34.628 | 12.663 | 102.469 | 1.00 | 47.74 |
| ATOM | 1610 | NZ | LYS | A | 202 | 33.504 | 12.290 | 103.378 | 1.00 | 53.56 |
| ATOM | 1611 | C | LYS | A | 202 | 40.382 | 15.101 | 102.753 | 1.00 | 36.27 |
| ATOM | 1612 | O | LYS | A | 202 | 41.520 | 14.666 | 102.613 | 1.00 | 28.06 |
| ATOM | 1613 | N | GLY | A | 203 | 40.080 | 16.152 | 103.509 | 1.00 | 31.91 |
| ATOM | 1614 | CA | GLY | A | 203 | 41.115 | 16.862 | 104.228 | 1.00 | 33.75 |
| ATOM | 1615 | C | GLY | A | 203 | 41.288 | 18.288 | 103.729 | 1.00 | 30.54 |
| ATOM | 1616 | O | GLY | A | 203 | 42.174 | 18.996 | 104.200 | 1.00 | 28.04 |
| ATOM | 1617 | N | PHE | A | 204 | 40.458 | 18.713 | 102.778 | 1.00 | 29.93 |
| ATOM | 1618 | CA | PHE | A | 204 | 40.557 | 20.077 | 102.260 | 1.00 | 35.76 |
| ATOM | 1619 | CB | PHE | A | 204 | 39.863 | 20.217 | 100.901 | 1.00 | 31.41 |
| ATOM | 1620 | CG | PHE | A | 204 | 40.498 | 19.416 | 99.803 | 1.00 | 31.06 |
| ATOM | 1621 | CD1 | PHE | A | 204 | 40.169 | 18.075 | 99.618 | 1.00 | 35.66 |
| ATOM | 1622 | CD2 | PHE | A | 204 | 41.431 | 20.002 | 98.955 | 1.00 | 30.79 |
| ATOM | 1623 | CE1 | PHE | A | 204 | 40.761 | 17.329 | 98.597 | 1.00 | 35.20 |
| ATOM | 1624 | CE2 | PHE | A | 204 | 42.033 | 19.267 | 97.931 | 1.00 | 36.08 |
| ATOM | 1625 | CZ | PHE | A | 204 | 41.697 | 17.928 | 97.751 | 1.00 | 36.54 |
| ATOM | 1626 | C | PHE | A | 204 | 39.967 | 21.103 | 103.231 | 1.00 | 37.30 |
| ATOM | 1627 | O | PHE | A | 204 | 39.088 | 20.786 | 104.040 | 1.00 | 33.56 |
| ATOM | 1628 | N | LEU | A | 205 | 40.451 | 22.337 | 103.128 | 1.00 | 38.52 |
| ATOM | 1629 | CA | LEU | A | 205 | 40.012 | 23.427 | 103.993 | 1.00 | 36.81 |
| ATOM | 1630 | CB | LEU | A | 205 | 40.801 | 24.695 | 103.659 | 1.00 | 34.73 |
| ATOM | 1631 | CG | LEU | A | 205 | 40.496 | 25.954 | 104.479 | 1.00 | 40.98 |
| ATOM | 1632 | CD1 | LEU | A | 205 | 40.690 | 25.677 | 105.965 | 1.00 | 39.87 |
| ATOM | 1633 | CD2 | LEU | A | 205 | 41.415 | 27.079 | 104.032 | 1.00 | 39.94 |
| ATOM | 1634 | C | LEU | A | 205 | 38.520 | 23.728 | 103.925 | 1.00 | 36.58 |
| ATOM | 1635 | O | LEU | A | 205 | 37.931 | 24.178 | 104.905 | 1.00 | 40.98 |
| ATOM | 1636 | N | GLU | A | 206 | 37.909 | 23.477 | 102.774 | 1.00 | 36.07 |
| ATOM | 1637 | CA | GLU | A | 206 | 36.486 | 23.748 | 102.586 | 1.00 | 36.30 |
| ATOM | 1638 | CB | GLU | A | 206 | 36.107 | 23.597 | 101.105 | 1.00 | 39.98 |
| ATOM | 1639 | CG | GLU | A | 206 | 36.890 | 24.473 | 100.131 | 1.00 | 48.04 |
| ATOM | 1640 | CD | GLU | A | 206 | 38.307 | 23.980 | 99.868 | 1.00 | 51.87 |
| ATOM | 1641 | OE1 | GLU | A | 206 | 39.146 | 23.993 | 100.792 | 1.00 | 50.32 |
| ATOM | 1642 | OE2 | GLU | A | 206 | 38.581 | 23.569 | 98.716 | 1.00 | 56.69 |
| ATOM | 1643 | C | GLU | A | 206 | 35.572 | 22.852 | 103.427 | 1.00 | 33.85 |
| ATOM | 1644 | O | GLU | A | 206 | 34.433 | 23.213 | 103.718 | 1.00 | 26.22 |
| ATOM | 1645 | N | GLU | A | 207 | 36.071 | 21.679 | 103.805 | 1.00 | 31.68 |
| ATOM | 1646 | CA | GLU | A | 207 | 35.297 | 20.726 | 104.599 | 1.00 | 31.65 |
| ATOM | 1647 | CB | GLU | A | 207 | 36.000 | 19.369 | 104.566 | 1.00 | 34.15 |
| ATOM | 1648 | CG | GLU | A | 207 | 36.044 | 18.741 | 103.179 | 1.00 | 33.80 |
| ATOM | 1649 | CD | GLU | A | 207 | 37.182 | 17.751 | 103.022 | 1.00 | 33.85 |
| ATOM | 1650 | OE1 | GLU | A | 207 | 37.487 | 17.025 | 103.995 | 1.00 | 33.22 |

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Figure 18-26

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1651 | OE2 | GLU | A | 207 | 37.760 | 17.688 | 101.916 | 1.00 | 35.48 |
| ATOM | 1652 | C | GLU | A | 207 | 35.182 | 21.229 | 106.033 | 1.00 | 35.06 |
| ATOM | 1653 | O | GLU | A | 207 | 36.009 | 20.894 | 106.887 | 1.00 | 34.16 |
| ATOM | 1654 | N | ILE | A | 208 | 34.150 | 22.024 | 106.302 | 1.00 | 35.99 |
| ATOM | 1655 | CA | ILE | A | 208 | 33.968 | 22.604 | 107.634 | 1.00 | 38.96 |
| ATOM | 1656 | CB | ILE | A | 208 | 33.737 | 24.134 | 107.529 | 1.00 | 42.74 |
| ATOM | 1657 | CG2 | ILE | A | 208 | 33.717 | 24.762 | 108.914 | 1.00 | 48.29 |
| ATOM | 1658 | CG1 | ILE | A | 208 | 34.841 | 24.795 | 106.700 | 1.00 | 40.34 |
| ATOM | 1659 | CD1 | ILE | A | 208 | 36.207 | 24.758 | 107.335 | 1.00 | 46.23 |
| ATOM | 1660 | C | ILE | A | 208 | 32.821 | 21.998 | 108.452 | 1.00 | 38.32 |
| ATOM | 1661 | O | ILE | A | 208 | 32.558 | 22.434 | 109.571 | 1.00 | 40.08 |
| ATOM | 1662 | N | GLY | A | 209 | 32.142 | 20.997 | 107.901 | 1.00 | 34.36 |
| ATOM | 1663 | CA | GLY | A | 209 | 31.047 | 20.374 | 108.620 | 1.00 | 33.32 |
| ATOM | 1664 | C | GLY | A | 209 | 29.699 | 20.673 | 107.993 | 1.00 | 37.87 |
| ATOM | 1665 | O | GLY | A | 209 | 29.579 | 21.581 | 107.173 | 1.00 | 40.56 |
| ATOM | 1666 | N | GLU | A | 210 | 28.676 | 19.917 | 108.380 | 1.00 | 37.38 |
| ATOM | 1667 | CA | GLU | A | 210 | 27.337 | 20.118 | 107.831 | 1.00 | 42.34 |
| ATOM | 1668 | CB | GLU | A | 210 | 27.008 | 19.012 | 106.823 | 1.00 | 42.73 |
| ATOM | 1669 | CG | GLU | A | 210 | 26.860 | 17.636 | 107.460 | 1.00 | 47.38 |
| ATOM | 1670 | CD | GLU | A | 210 | 26.633 | 16.532 | 106.443 | 1.00 | 52.68 |
| ATOM | 1671 | OE1 | GLU | A | 210 | 26.385 | 15.379 | 106.860 | 1.00 | 50.59 |
| ATOM | 1672 | OE2 | GLU | A | 210 | 26.711 | 16.810 | 105.226 | 1.00 | 53.78 |
| ATOM | 1673 | C | GLU | A | 210 | 26.287 | 20.114 | 108.938 | 1.00 | 42.90 |
| ATOM | 1674 | O | GLU | A | 210 | 26.516 | 19.577 | 110.022 | 1.00 | 45.94 |
| ATOM | 1675 | N | GLY | A | 211 | 25.130 | 20.702 | 108.654 | 1.00 | 43.16 |
| ATOM | 1676 | CA | GLY | A | 211 | 24.068 | 20.751 | 109.642 | 1.00 | 43.98 |
| ATOM | 1677 | C | GLY | A | 211 | 24.514 | 21.450 | 110.911 | 1.00 | 45.01 |
| ATOM | 1678 | O | GLY | A | 211 | 25.186 | 22.479 | 110.858 | 1.00 | 48.15 |
| ATOM | 1679 | N | LYS | A | 212 | 24.145 | 20.896 | 112.059 | 1.00 | 41.63 |
| ATOM | 1680 | CA | LYS | A | 212 | 24.528 | 21.495 | 113.328 | 1.00 | 45.07 |
| ATOM | 1681 | CB | LYS | A | 212 | 23.913 | 20.715 | 114.490 | 1.00 | 46.59 |
| ATOM | 1682 | CG | LYS | A | 212 | 22.386 | 20.591 | 114.462 | 1.00 | 55.31 |
| ATOM | 1683 | CD | LYS | A | 212 | 21.651 | 21.945 | 114.481 | 1.00 | 57.42 |
| ATOM | 1684 | CE | LYS | A | 212 | 21.749 | 22.696 | 113.151 | 1.00 | 59.71 |
| ATOM | 1685 | NZ | LYS | A | 212 | 21.051 | 24.017 | 113.178 | 1.00 | 57.43 |
| ATOM | 1686 | C | LYS | A | 212 | 26.046 | 21.513 | 113.469 | 1.00 | 42.08 |
| ATOM | 1687 | O | LYS | A | 212 | 26.598 | 22.326 | 114.207 | 1.00 | 40.03 |
| ATOM | 1688 | N | GLY | A | 213 | 26.713 | 20.615 | 112.751 | 1.00 | 39.51 |
| ATOM | 1689 | CA | GLY | A | 213 | 28.163 | 20.538 | 112.817 | 1.00 | 40.11 |
| ATOM | 1690 | C | GLY | A | 213 | 28.888 | 21.519 | 111.916 | 1.00 | 38.25 |
| ATOM | 1691 | O | GLY | A | 213 | 30.122 | 21.575 | 111.913 | 1.00 | 34.70 |
| ATOM | 1692 | N | LYS | A | 214 | 28.131 | 22.295 | 111.143 | 1.00 | 37.31 |
| ATOM | 1693 | CA | LYS | A | 214 | 28.736 | 23.274 | 110.250 | 1.00 | 39.58 |
| ATOM | 1694 | CB | LYS | A | 214 | 27.656 | 24.017 | 109.463 | 1.00 | 44.69 |
| ATOM | 1695 | CG | LYS | A | 214 | 28.189 | 25.030 | 108.461 | 1.00 | 44.53 |
| ATOM | 1696 | CD | LYS | A | 214 | 27.047 | 25.704 | 107.720 | 1.00 | 47.71 |
| ATOM | 1697 | CE | LYS | A | 214 | 27.553 | 26.759 | 106.754 | 1.00 | 52.94 |
| ATOM | 1698 | NZ | LYS | A | 214 | 28.453 | 26.183 | 105.717 | 1.00 | 57.45 |
| ATOM | 1699 | C | LYS | A | 214 | 29.547 | 24.259 | 111.085 | 1.00 | 40.16 |
| ATOM | 1700 | O | LYS | A | 214 | 29.002 | 24.963 | 111.933 | 1.00 | 37.92 |
| ATOM | 1701 | N | GLY | A | 215 | 30.851 | 24.295 | 110.846 | 1.00 | 36.57 |
| ATOM | 1702 | CA | GLY | A | 215 | 31.716 | 25.183 | 111.593 | 1.00 | 35.03 |
| ATOM | 1703 | C | GLY | A | 215 | 32.431 | 24.448 | 112.709 | 1.00 | 34.57 |
| ATOM | 1704 | O | GLY | A | 215 | 33.216 | 25.039 | 113.454 | 1.00 | 33.76 |
| ATOM | 1705 | N | TYR | A | 216 | 32.168 | 23.153 | 112.837 | 1.00 | 34.61 |
| ATOM | 1706 | CA | TYR | A | 216 | 32.816 | 22.378 | 113.885 | 1.00 | 35.00 |
| ATOM | 1707 | CB | TYR | A | 216 | 31.763 | 21.683 | 114.753 | 1.00 | 36.19 |
| ATOM | 1708 | CG | TYR | A | 216 | 30.928 | 22.671 | 115.547 | 1.00 | 36.68 |
| ATOM | 1709 | CD1 | TYR | A | 216 | 29.961 | 23.462 | 114.925 | 1.00 | 35.83 |
| ATOM | 1710 | CE1 | TYR | A | 216 | 29.249 | 24.431 | 115.641 | 1.00 | 40.89 |
| ATOM | 1711 | CD2 | TYR | A | 216 | 31.163 | 22.869 | 116.910 | 1.00 | 41.50 |
| ATOM | 1712 | CE2 | TYR | A | 216 | 30.459 | 23.834 | 117.634 | 1.00 | 40.69 |
| ATOM | 1713 | CZ | TYR | A | 216 | 29.505 | 24.612 | 116.994 | 1.00 | 40.17 |
| ATOM | 1714 | OH | TYR | A | 216 | 28.816 | 25.566 | 117.708 | 1.00 | 38.09 |
| ATOM | 1715 | C | TYR | A | 216 | 33.877 | 21.384 | 113.401 | 1.00 | 34.05 |
| ATOM | 1716 | O | TYR | A | 216 | 34.263 | 20.462 | 114.127 | 1.00 | 31.87 |

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Figure 18-27

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 1717 | N | ASN A 217 | 34.343 | 21.580 | 112.170 | 1.00 | 29.90 |
| ATOM | 1718 | CA | ASN A 217 | 35.398 | 20.748 | 111.606 | 1.00 | 30.02 |
| ATOM | 1719 | CB | ASN A 217 | 34.833 | 19.727 | 110.615 | 1.00 | 26.46 |
| ATOM | 1720 | CG | ASN A 217 | 35.897 | 18.764 | 110.105 | 1.00 | 30.13 |
| ATOM | 1721 | OD1 | ASN A 217 | 36.558 | 19.022 | 109.097 | 1.00 | 29.80 |
| ATOM | 1722 | ND2 | ASN A 217 | 36.094 | 17.659 | 110.831 | 1.00 | 19.92 |
| ATOM | 1723 | C | ASN A 217 | 36.378 | 21.686 | 110.915 | 1.00 | 30.23 |
| ATOM | 1724 | O | ASN A 217 | 35.983 | 22.502 | 110.080 | 1.00 | 27.88 |
| ATOM | 1725 | N | LEU A 218 | 37.655 | 21.577 | 111.271 | 1.00 | 29.45 |
| ATOM | 1726 | CA | LEU A 218 | 38.670 | 22.451 | 110.698 | 1.00 | 28.76 |
| ATOM | 1727 | CB | LEU A 218 | 39.160 | 23.444 | 111.753 | 1.00 | 29.02 |
| ATOM | 1728 | CG | LEU A 218 | 39.513 | 24.867 | 111.307 | 1.00 | 34.69 |
| ATOM | 1729 | CD1 | LEU A 218 | 40.432 | 25.480 | 112.367 | 1.00 | 32.93 |
| ATOM | 1730 | CD2 | LEU A 218 | 40.197 | 24.873 | 109.954 | 1.00 | 30.69 |
| ATOM | 1731 | C | LEU A 218 | 39.870 | 21.657 | 110.207 | 1.00 | 26.65 |
| ATOM | 1732 | O | LEU A 218 | 40.527 | 20.981 | 110.999 | 1.00 | 25.25 |
| ATOM | 1733 | N | ASN A 219 | 40.151 | 21.752 | 108.909 | 1.00 | 25.21 |
| ATOM | 1734 | CA | ASN A 219 | 41.287 | 21.069 | 108.294 | 1.00 | 21.91 |
| ATOM | 1735 | CB | ASN A 219 | 40.875 | 20.314 | 107.018 | 1.00 | 23.69 |
| ATOM | 1736 | CG | ASN A 219 | 39.972 | 19.144 | 107.298 | 1.00 | 27.88 |
| ATOM | 1737 | OD1 | ASN A 219 | 40.153 | 18.440 | 108.289 | 1.00 | 29.28 |
| ATOM | 1738 | ND2 | ASN A 219 | 39.018 | 18.900 | 106.407 | 1.00 | 24.48 |
| ATOM | 1739 | C | ASN A 219 | 42.355 | 22.074 | 107.906 | 1.00 | 23.46 |
| ATOM | 1740 | O | ASN A 219 | 42.059 | 23.073 | 107.259 | 1.00 | 28.17 |
| ATOM | 1741 | N | ILE A 220 | 43.595 | 21.804 | 108.287 | 1.00 | 23.90 |
| ATOM | 1742 | CA | ILE A 220 | 44.702 | 22.684 | 107.945 | 1.00 | 23.22 |
| ATOM | 1743 | CB | ILE A 220 | 45.468 | 23.131 | 109.212 | 1.00 | 28.73 |
| ATOM | 1744 | CG2 | ILE A 220 | 46.601 | 24.078 | 108.831 | 1.00 | 26.01 |
| ATOM | 1745 | CG1 | ILE A 220 | 44.502 | 23.783 | 110.212 | 1.00 | 26.36 |
| ATOM | 1746 | CD1 | ILE A 220 | 43.771 | 25.004 | 109.688 | 1.00 | 25.74 |
| ATOM | 1747 | C | ILE A 220 | 45.669 | 21.929 | 107.018 | 1.00 | 25.29 |
| ATOM | 1748 | O | ILE A 220 | 46.631 | 21.315 | 107.477 | 1.00 | 20.44 |
| ATOM | 1749 | N | PRO A 221 | 45.396 | 21.924 | 105.703 | 1.00 | 26.34 |
| ATOM | 1750 | CD | PRO A 221 | 44.234 | 22.497 | 104.999 | 1.00 | 28.22 |
| ATOM | 1751 | CA | PRO A 221 | 46.271 | 21.234 | 104.747 | 1.00 | 26.92 |
| ATOM | 1752 | CB | PRO A 221 | 45.454 | 21.279 | 103.457 | 1.00 | 27.81 |
| ATOM | 1753 | CG | PRO A 221 | 44.774 | 22.622 | 103.582 | 1.00 | 30.62 |
| ATOM | 1754 | C | PRO A 221 | 47.595 | 21.977 | 104.625 | 1.00 | 27.45 |
| ATOM | 1755 | O | PRO A 221 | 47.603 | 23.199 | 104.457 | 1.00 | 31.21 |
| ATOM | 1756 | N | LEU A 222 | 48.704 | 21.242 | 104.703 | 1.00 | 26.01 |
| ATOM | 1757 | CA | LEU A 222 | 50.038 | 21.838 | 104.640 | 1.00 | 26.41 |
| ATOM | 1758 | CB | LEU A 222 | 50.726 | 21.650 | 105.997 | 1.00 | 26.12 |
| ATOM | 1759 | CG | LEU A 222 | 49.960 | 22.322 | 107.150 | 1.00 | 27.67 |
| ATOM | 1760 | CD1 | LEU A 222 | 50.531 | 21.899 | 108.497 | 1.00 | 30.97 |
| ATOM | 1761 | CD2 | LEU A 222 | 50.024 | 23.839 | 106.985 | 1.00 | 31.59 |
| ATOM | 1762 | C | LEU A 222 | 50.911 | 21.286 | 103.504 | 1.00 | 28.97 |
| ATOM | 1763 | O | LEU A 222 | 50.784 | 20.128 | 103.117 | 1.00 | 27.95 |
| ATOM | 1764 | N | PRO A 223 | 51.821 | 22.116 | 102.964 | 1.00 | 31.52 |
| ATOM | 1765 | CD | PRO A 223 | 52.059 | 23.518 | 103.358 | 1.00 | 29.08 |
| ATOM | 1766 | CA | PRO A 223 | 52.727 | 21.753 | 101.865 | 1.00 | 29.93 |
| ATOM | 1767 | CB | PRO A 223 | 53.265 | 23.109 | 101.428 | 1.00 | 29.16 |
| ATOM | 1768 | CG | PRO A 223 | 53.458 | 23.771 | 102.779 | 1.00 | 25.86 |
| ATOM | 1769 | C | PRO A 223 | 53.862 | 20.782 | 102.206 | 1.00 | 33.62 |
| ATOM | 1770 | O | PRO A 223 | 54.179 | 20.531 | 103.376 | 1.00 | 26.55 |
| ATOM | 1771 | N | LYS A 224 | 54.479 | 20.257 | 101.153 | 1.00 | 34.00 |
| ATOM | 1772 | CA | LYS A 224 | 55.595 | 19.320 | 101.264 | 1.00 | 32.88 |
| ATOM | 1773 | CB | LYS A 224 | 55.938 | 18.767 | 99.884 | 1.00 | 36.31 |
| ATOM | 1774 | CG | LYS A 224 | 54.761 | 18.204 | 99.115 | 1.00 | 39.37 |
| ATOM | 1775 | CD | LYS A 224 | 55.150 | 17.998 | 97.658 | 1.00 | 45.23 |
| ATOM | 1776 | CE | LYS A 224 | 53.989 | 17.478 | 96.835 | 1.00 | 47.90 |
| ATOM | 1777 | NZ | LYS A 224 | 54.331 | 17.441 | 95.388 | 1.00 | 46.60 |
| ATOM | 1778 | C | LYS A 224 | 56.817 | 20.054 | 101.798 | 1.00 | 29.43 |
| ATOM | 1779 | O | LYS A 224 | 56.933 | 21.270 | 101.640 | 1.00 | 24.10 |
| ATOM | 1780 | N | GLY A 225 | 57.735 | 19.305 | 102.403 | 1.00 | 25.00 |
| ATOM | 1781 | CA | GLY A 225 | 58.947 | 19.896 | 102.942 | 1.00 | 26.20 |
| ATOM | 1782 | C | GLY A 225 | 58.727 | 20.792 | 104.154 | 1.00 | 29.44 |

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Figure 18-28

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 1783 | O | GLY A 225 | 59.610 | 21.562 | 104.528 | 1.00 | 29.09 |
| ATOM | 1784 | N | LEU A 226 | 57.560 | 20.679 | 104.777 | 1.00 | 24.26 |
| ATOM | 1785 | CA | LEU A 226 | 57.212 | 21.488 | 105.951 | 1.00 | 25.35 |
| ATOM | 1786 | CB | LEU A 226 | 55.930 | 20.925 | 106.579 | 1.00 | 23.23 |
| ATOM | 1787 | CG | LEU A 226 | 55.172 | 21.757 | 107.611 | 1.00 | 28.28 |
| ATOM | 1788 | CD1 | LEU A 226 | 54.596 | 22.972 | 106.911 | 1.00 | 28.07 |
| ATOM | 1789 | CD2 | LEU A 226 | 54.036 | 20.933 | 108.226 | 1.00 | 27.49 |
| ATOM | 1790 | C | LEU A 226 | 58.333 | 21.501 | 106.998 | 1.00 | 24.79 |
| ATOM | 1791 | O | LEU A 226 | 58.902 | 20.450 | 107.299 | 1.00 | 26.15 |
| ATOM | 1792 | N | ASN A 227 | 58.664 | 22.674 | 107.548 | 1.00 | 23.94 |
| ATOM | 1793 | CA | ASN A 227 | 59.702 | 22.733 | 108.578 | 1.00 | 24.89 |
| ATOM | 1794 | CB | ASN A 227 | 60.751 | 23.823 | 108.269 | 1.00 | 27.43 |
| ATOM | 1795 | CG | ASN A 227 | 60.190 | 25.231 | 108.334 | 1.00 | 31.62 |
| ATOM | 1796 | OD1 | ASN A 227 | 59.598 | 25.632 | 109.336 | 1.00 | 31.17 |
| ATOM | 1797 | ND2 | ASN A 227 | 60.395 | 25.998 | 107.267 | 1.00 | 28.06 |
| ATOM | 1798 | C | ASN A 227 | 59.076 | 22.957 | 109.960 | 1.00 | 23.16 |
| ATOM | 1799 | O | ASN A 227 | 57.873 | 23.206 | 110.065 | 1.00 | 18.45 |
| ATOM | 1800 | N | ASP A 228 | 59.880 | 22.862 | 111.018 | 1.00 | 21.29 |
| ATOM | 1801 | CA | ASP A 228 | 59.357 | 23.032 | 112.375 | 1.00 | 25.80 |
| ATOM | 1802 | CB | ASP A 228 | 60.464 | 22.893 | 113.426 | 1.00 | 24.02 |
| ATOM | 1803 | CG | ASP A 228 | 61.110 | 21.520 | 113.422 | 1.00 | 26.48 |
| ATOM | 1804 | OD1 | ASP A 228 | 60.410 | 20.530 | 113.135 | 1.00 | 29.55 |
| ATOM | 1805 | OD2 | ASP A 228 | 62.311 | 21.425 | 113.744 | 1.00 | 29.88 |
| ATOM | 1806 | C | ASP A 228 | 58.628 | 24.341 | 112.620 | 1.00 | 27.83 |
| ATOM | 1807 | O | ASP A 228 | 57.589 | 24.360 | 113.284 | 1.00 | 25.68 |
| ATOM | 1808 | N | ASN A 229 | 59.167 | 25.437 | 112.098 | 1.00 | 25.78 |
| ATOM | 1809 | CA | ASN A 229 | 58.537 | 26.739 | 112.297 | 1.00 | 27.75 |
| ATOM | 1810 | CB | ASN A 229 | 59.453 | 27.850 | 111.770 | 1.00 | 32.77 |
| ATOM | 1811 | CG | ASN A 229 | 60.707 | 28.020 | 112.621 | 1.00 | 30.35 |
| ATOM | 1812 | OD1 | ASN A 229 | 60.635 | 28.433 | 113.782 | 1.00 | 33.12 |
| ATOM | 1813 | ND2 | ASN A 229 | 61.856 | 27.691 | 112.053 | 1.00 | 28.11 |
| ATOM | 1814 | C | ASN A 229 | 57.168 | 26.817 | 111.645 | 1.00 | 29.47 |
| ATOM | 1815 | O | ASN A 229 | 56.230 | 27.387 | 112.202 | 1.00 | 26.75 |
| ATOM | 1816 | N | GLU A 230 | 57.041 | 26.228 | 110.463 | 1.00 | 30.80 |
| ATOM | 1817 | CA | GLU A 230 | 55.761 | 26.244 | 109.773 | 1.00 | 30.77 |
| ATOM | 1818 | CB | GLU A 230 | 55.929 | 25.716 | 108.341 | 1.00 | 29.11 |
| ATOM | 1819 | CG | GLU A 230 | 56.897 | 26.531 | 107.507 | 1.00 | 35.94 |
| ATOM | 1820 | CD | GLU A 230 | 57.119 | 25.946 | 106.125 | 1.00 | 37.77 |
| ATOM | 1821 | OE1 | GLU A 230 | 57.465 | 24.748 | 106.039 | 1.00 | 38.98 |
| ATOM | 1822 | OE2 | GLU A 230 | 56.957 | 26.684 | 105.129 | 1.00 | 31.32 |
| ATOM | 1823 | C | GLU A 230 | 54.723 | 25.407 | 110.527 | 1.00 | 30.13 |
| ATOM | 1824 | O | GLU A 230 | 53.563 | 25.799 | 110.631 | 1.00 | 28.35 |
| ATOM | 1825 | N | PHE A 231 | 55.141 | 24.262 | 111.060 | 1.00 | 32.49 |
| ATOM | 1826 | CA | PHE A 231 | 54.223 | 23.386 | 111.790 | 1.00 | 28.54 |
| ATOM | 1827 | CB | PHE A 231 | 54.913 | 22.075 | 112.191 | 1.00 | 31.22 |
| ATOM | 1828 | CG | PHE A 231 | 53.974 | 21.050 | 112.781 | 1.00 | 28.41 |
| ATOM | 1829 | CD1 | PHE A 231 | 53.026 | 20.417 | 111.982 | 1.00 | 29.66 |
| ATOM | 1830 | CD2 | PHE A 231 | 54.036 | 20.723 | 114.130 | 1.00 | 28.38 |
| ATOM | 1831 | CE1 | PHE A 231 | 52.153 | 19.469 | 112.518 | 1.00 | 25.79 |
| ATOM | 1832 | CE2 | PHE A 231 | 53.166 | 19.774 | 114.681 | 1.00 | 31.40 |
| ATOM | 1833 | CZ | PHE A 231 | 52.223 | 19.146 | 113.870 | 1.00 | 30.51 |
| ATOM | 1834 | C | PHE A 231 | 53.693 | 24.065 | 113.045 | 1.00 | 26.85 |
| ATOM | 1835 | O | PHE A 231 | 52.483 | 24.092 | 113.277 | 1.00 | 25.99 |
| ATOM | 1836 | N | LEU A 232 | 54.598 | 24.607 | 113.858 | 1.00 | 26.75 |
| ATOM | 1837 | CA | LEU A 232 | 54.193 | 25.283 | 115.092 | 1.00 | 27.25 |
| ATOM | 1838 | CB | LEU A 232 | 55.422 | 25.617 | 115.933 | 1.00 | 25.15 |
| ATOM | 1839 | CG | LEU A 232 | 56.176 | 24.372 | 116.420 | 1.00 | 28.11 |
| ATOM | 1840 | CD1 | LEU A 232 | 57.440 | 24.783 | 117.162 | 1.00 | 27.32 |
| ATOM | 1841 | CD2 | LEU A 232 | 55.268 | 23.540 | 117.328 | 1.00 | 27.87 |
| ATOM | 1842 | C | LEU A 232 | 53.371 | 26.542 | 114.800 | 1.00 | 26.98 |
| ATOM | 1843 | O | LEU A 232 | 52.449 | 26.866 | 115.544 | 1.00 | 23.34 |
| ATOM | 1844 | N | PHE A 233 | 53.694 | 27.232 | 113.708 | 1.00 | 24.99 |
| ATOM | 1845 | CA | PHE A 233 | 52.950 | 28.426 | 113.312 | 1.00 | 28.13 |
| ATOM | 1846 | CB | PHE A 233 | 53.542 | 29.029 | 112.029 | 1.00 | 30.77 |
| ATOM | 1847 | CG | PHE A 233 | 52.719 | 30.151 | 111.448 | 1.00 | 29.65 |
| ATOM | 1848 | CD1 | PHE A 233 | 52.803 | 31.441 | 111.962 | 1.00 | 32.80 |

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Figure 18-29

| | | | | | | | |
|------|------|----------------|--------|--------|---------|------|-------|
| ATOM | 1849 | CD2. PHE A 233 | 51.825 | 29.903 | 110.412 | 1.00 | 31.59 |
| ATOM | 1850 | CE1 PHE A 233 | 52.008 | 32.468 | 111.452 | 1.00 | 33.90 |
| ATOM | 1851 | CE2 PHE A 233 | 51.022 | 30.924 | 109.895 | 1.00 | 32.47 |
| ATOM | 1852 | CZ PHE A 233 | 51.114 | 32.208 | 110.415 | 1.00 | 32.50 |
| ATOM | 1853 | C PHE A 233 | 51.510 | 27.999 | 113.031 | 1.00 | 31.62 |
| ATOM | 1854 | O PHE A 233 | 50.553 | 28.603 | 113.532 | 1.00 | 25.88 |
| ATOM | 1855 | N ALA A 234 | 51.370 | 26.955 | 112.215 | 1.00 | 28.12 |
| ATOM | 1856 | CA ALA A 234 | 50.056 | 26.436 | 111.853 | 1.00 | 25.68 |
| ATOM | 1857 | CB ALA A 234 | 50.195 | 25.279 | 110.864 | 1.00 | 20.08 |
| ATOM | 1858 | C ALA A 234 | 49.304 | 25.969 | 113.089 | 1.00 | 25.17 |
| ATOM | 1859 | O ALA A 234 | 48.114 | 26.228 | 113.234 | 1.00 | 25.21 |
| ATOM | 1860 | N LEU A 235 | 50.002 | 25.285 | 113.987 | 1.00 | 28.18 |
| ATOM | 1861 | CA LEU A 235 | 49.367 | 24.781 | 115.195 | 1.00 | 33.70 |
| ATOM | 1862 | CB LEU A 235 | 50.356 | 23.964 | 116.026 | 1.00 | 32.70 |
| ATOM | 1863 | CG LEU A 235 | 49.772 | 22.788 | 116.820 | 1.00 | 36.89 |
| ATOM | 1864 | CD1 LEU A 235 | 50.634 | 22.545 | 118.052 | 1.00 | 31.37 |
| ATOM | 1865 | CD2 LEU A 235 | 48.344 | 23.072 | 117.231 | 1.00 | 31.47 |
| ATOM | 1866 | C LEU A 235 | 48.841 | 25.925 | 116.062 | 1.00 | 33.38 |
| ATOM | 1867 | O LEU A 235 | 47.673 | 25.926 | 116.455 | 1.00 | 28.13 |
| ATOM | 1868 | N GLU A 236 | 49.710 | 26.888 | 116.362 | 1.00 | 34.02 |
| ATOM | 1869 | CA GLU A 236 | 49.336 | 28.026 | 117.199 | 1.00 | 37.30 |
| ATOM | 1870 | CB GLU A 236 | 50.528 | 28.972 | 117.400 | 1.00 | 41.51 |
| ATOM | 1871 | CG GLU A 236 | 51.675 | 28.356 | 118.188 | 1.00 | 49.54 |
| ATOM | 1872 | CD GLU A 236 | 52.811 | 29.334 | 118.451 | 1.00 | 55.02 |
| ATOM | 1873 | OE1 GLU A 236 | 53.781 | 28.947 | 119.140 | 1.00 | 56.19 |
| ATOM | 1874 | OE2 GLU A 236 | 52.735 | 30.486 | 117.968 | 1.00 | 54.84 |
| ATOM | 1875 | C GLU A 236 | 48.163 | 28.803 | 116.638 | 1.00 | 33.98 |
| ATOM | 1876 | O GLU A 236 | 47.211 | 29.098 | 117.362 | 1.00 | 37.01 |
| ATOM | 1877 | N LYS A 237 | 48.223 | 29.137 | 115.354 | 1.00 | 33.94 |
| ATOM | 1878 | CA LYS A 237 | 47.140 | 29.888 | 114.726 | 1.00 | 33.10 |
| ATOM | 1879 | CB LYS A 237 | 47.505 | 30.244 | 113.281 | 1.00 | 36.08 |
| ATOM | 1880 | CG LYS A 237 | 48.695 | 31.186 | 113.165 | 1.00 | 33.62 |
| ATOM | 1881 | CD LYS A 237 | 48.395 | 32.508 | 113.856 | 1.00 | 37.99 |
| ATOM | 1882 | CE LYS A 237 | 49.569 | 33.471 | 113.762 | 1.00 | 45.24 |
| ATOM | 1883 | NZ LYS A 237 | 49.285 | 34.737 | 114.500 | 1.00 | 43.49 |
| ATOM | 1884 | C LYS A 237 | 45.820 | 29.128 | 114.751 | 1.00 | 31.40 |
| ATOM | 1885 | O LYS A 237 | 44.793 | 29.680 | 115.131 | 1.00 | 31.67 |
| ATOM | 1886 | N SER A 238 | 45.841 | 27.861 | 114.354 | 1.00 | 28.72 |
| ATOM | 1887 | CA SER A 238 | 44.610 | 27.080 | 114.335 | 1.00 | 31.74 |
| ATOM | 1888 | CB SER A 238 | 44.834 | 25.720 | 113.660 | 1.00 | 28.90 |
| ATOM | 1889 | OG SER A 238 | 45.760 | 24.924 | 114.372 | 1.00 | 25.18 |
| ATOM | 1890 | C SER A 238 | 44.041 | 26.891 | 115.740 | 1.00 | 33.23 |
| ATOM | 1891 | O SER A 238 | 42.823 | 26.875 | 115.916 | 1.00 | 34.79 |
| ATOM | 1892 | N LEU A 239 | 44.907 | 26.742 | 116.741 | 1.00 | 35.27 |
| ATOM | 1893 | CA LEU A 239 | 44.413 | 26.587 | 118.108 | 1.00 | 37.57 |
| ATOM | 1894 | CB LEU A 239 | 45.554 | 26.307 | 119.090 | 1.00 | 38.58 |
| ATOM | 1895 | CG LEU A 239 | 46.176 | 24.907 | 119.038 | 1.00 | 39.74 |
| ATOM | 1896 | CD1 LEU A 239 | 47.276 | 24.797 | 120.075 | 1.00 | 35.82 |
| ATOM | 1897 | CD2 LEU A 239 | 45.109 | 23.861 | 119.301 | 1.00 | 34.93 |
| ATOM | 1898 | C LEU A 239 | 43.670 | 27.852 | 118.521 | 1.00 | 39.09 |
| ATOM | 1899 | O LEU A 239 | 42.628 | 27.782 | 119.174 | 1.00 | 35.50 |
| ATOM | 1900 | N GLU A 240 | 44.202 | 29.007 | 118.131 | 1.00 | 39.27 |
| ATOM | 1901 | CA GLU A 240 | 43.561 | 30.281 | 118.450 | 1.00 | 40.15 |
| ATOM | 1902 | CB GLU A 240 | 44.366 | 31.448 | 117.883 | 1.00 | 40.42 |
| ATOM | 1903 | CG GLU A 240 | 45.661 | 31.747 | 118.602 | 1.00 | 43.91 |
| ATOM | 1904 | CD GLU A 240 | 46.407 | 32.884 | 117.942 | 1.00 | 49.31 |
| ATOM | 1905 | OE1 GLU A 240 | 45.772 | 33.925 | 117.665 | 1.00 | 49.00 |
| ATOM | 1906 | OE2 GLU A 240 | 47.624 | 32.745 | 117.705 | 1.00 | 54.05 |
| ATOM | 1907 | C GLU A 240 | 42.165 | 30.312 | 117.849 | 1.00 | 39.58 |
| ATOM | 1908 | O GLU A 240 | 41.224 | 30.822 | 118.455 | 1.00 | 40.99 |
| ATOM | 1909 | N ILE A 241 | 42.039 | 29.764 | 116.645 | 1.00 | 35.70 |
| ATOM | 1910 | CA ILE A 241 | 40.754 | 29.726 | 115.964 | 1.00 | 38.23 |
| ATOM | 1911 | CB ILE A 241 | 40.904 | 29.150 | 114.546 | 1.00 | 37.55 |
| ATOM | 1912 | CG2 ILE A 241 | 39.535 | 29.005 | 113.895 | 1.00 | 37.30 |
| ATOM | 1913 | CG1 ILE A 241 | 41.832 | 30.048 | 113.724 | 1.00 | 38.36 |
| ATOM | 1914 | CD1 ILE A 241 | 42.106 | 29.541 | 112.320 | 1.00 | 36.15 |

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Figure 18-30

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 1915 | C | ILE A 241 | 39.751 | 28.881 | 116.737 | 1.00 | 37.31 |
| ATOM | 1916 | O | ILE A 241 | 38.591 | 29.264 | 116.884 | 1.00 | 37.91 |
| ATOM | 1917 | N | VAL A 242 | 40.203 | 27.732 | 117.231 | 1.00 | 37.07 |
| ATOM | 1918 | CA | VAL A 242 | 39.336 | 26.832 | 117.981 | 1.00 | 38.35 |
| ATOM | 1919 | CB | VAL A 242 | 40.025 | 25.477 | 118.250 | 1.00 | 37.58 |
| ATOM | 1920 | CG1 | VAL A 242 | 39.120 | 24.581 | 119.078 | 1.00 | 31.91 |
| ATOM | 1921 | CG2 | VAL A 242 | 40.364 | 24.803 | 116.928 | 1.00 | 39.21 |
| ATOM | 1922 | C | VAL A 242 | 38.930 | 27.451 | 119.305 | 1.00 | 40.40 |
| ATOM | 1923 | O | VAL A 242 | 37.759 | 27.422 | 119.675 | 1.00 | 38.19 |
| ATOM | 1924 | N | LYS A 243 | 39.905 | 28.008 | 120.014 | 1.00 | 45.47 |
| ATOM | 1925 | CA | LYS A 243 | 39.661 | 28.654 | 121.301 | 1.00 | 48.74 |
| ATOM | 1926 | CB | LYS A 243 | 40.945 | 29.319 | 121.801 | 1.00 | 51.01 |
| ATOM | 1927 | CG | LYS A 243 | 41.853 | 28.426 | 122.614 | 1.00 | 56.09 |
| ATOM | 1928 | CD | LYS A 243 | 41.250 | 28.149 | 123.991 | 1.00 | 57.39 |
| ATOM | 1929 | CE | LYS A 243 | 41.054 | 29.436 | 124.783 | 1.00 | 59.53 |
| ATOM | 1930 | NZ | LYS A 243 | 40.448 | 29.193 | 126.127 | 1.00 | 57.91 |
| ATOM | 1931 | C | LYS A 243 | 38.559 | 29.705 | 121.260 | 1.00 | 51.67 |
| ATOM | 1932 | O | LYS A 243 | 37.815 | 29.871 | 122.226 | 1.00 | 52.84 |
| ATOM | 1933 | N | GLU A 244 | 38.451 | 30.410 | 120.140 | 1.00 | 53.77 |
| ATOM | 1934 | CA | GLU A 244 | 37.460 | 31.471 | 120.004 | 1.00 | 54.74 |
| ATOM | 1935 | CB | GLU A 244 | 37.954 | 32.497 | 118.986 | 1.00 | 55.15 |
| ATOM | 1936 | CG | GLU A 244 | 37.068 | 33.717 | 118.865 | 1.00 | 60.63 |
| ATOM | 1937 | CD | GLU A 244 | 37.602 | 34.714 | 117.868 | 1.00 | 65.87 |
| ATOM | 1938 | OE1 | GLU A 244 | 38.746 | 35.181 | 118.053 | 1.00 | 70.36 |
| ATOM | 1939 | OE2 | GLU A 244 | 36.879 | 35.031 | 116.900 | 1.00 | 67.09 |
| ATOM | 1940 | C | GLU A 244 | 36.051 | 31.025 | 119.626 | 1.00 | 52.65 |
| ATOM | 1941 | O | GLU A 244 | 35.127 | 31.838 | 119.606 | 1.00 | 55.59 |
| ATOM | 1942 | N | VAL A 245 | 35.869 | 29.745 | 119.332 | 1.00 | 50.57 |
| ATOM | 1943 | CA | VAL A 245 | 34.546 | 29.269 | 118.947 | 1.00 | 45.75 |
| ATOM | 1944 | CB | VAL A 245 | 34.475 | 29.081 | 117.409 | 1.00 | 46.91 |
| ATOM | 1945 | CG1 | VAL A 245 | 33.085 | 28.634 | 116.986 | 1.00 | 52.62 |
| ATOM | 1946 | CG2 | VAL A 245 | 34.825 | 30.389 | 116.716 | 1.00 | 48.34 |
| ATOM | 1947 | C | VAL A 245 | 34.130 | 27.969 | 119.642 | 1.00 | 42.67 |
| ATOM | 1948 | O | VAL A 245 | 33.021 | 27.480 | 119.445 | 1.00 | 43.61 |
| ATOM | 1949 | N | PHE A 246 | 35.001 | 27.417 | 120.477 | 1.00 | 40.87 |
| ATOM | 1950 | CA | PHE A 246 | 34.662 | 26.168 | 121.139 | 1.00 | 37.47 |
| ATOM | 1951 | CB | PHE A 246 | 35.106 | 24.991 | 120.257 | 1.00 | 37.00 |
| ATOM | 1952 | CG | PHE A 246 | 34.450 | 23.685 | 120.604 | 1.00 | 33.22 |
| ATOM | 1953 | CD1 | PHE A 246 | 33.111 | 23.467 | 120.302 | 1.00 | 33.93 |
| ATOM | 1954 | CD2 | PHE A 246 | 35.168 | 22.674 | 121.234 | 1.00 | 32.13 |
| ATOM | 1955 | CE1 | PHE A 246 | 32.493 | 22.260 | 120.621 | 1.00 | 37.75 |
| ATOM | 1956 | CE2 | PHE A 246 | 34.561 | 21.459 | 121.561 | 1.00 | 35.92 |
| ATOM | 1957 | CZ | PHE A 246 | 33.217 | 21.252 | 121.251 | 1.00 | 36.30 |
| ATOM | 1958 | C | PHE A 246 | 35.322 | 26.065 | 122.509 | 1.00 | 38.93 |
| ATOM | 1959 | O | PHE A 246 | 36.546 | 26.158 | 122.630 | 1.00 | 40.66 |
| ATOM | 1960 | N | GLU A 247 | 34.500 | 25.870 | 123.537 | 1.00 | 38.59 |
| ATOM | 1961 | CA | GLU A 247 | 34.970 | 25.733 | 124.918 | 1.00 | 44.60 |
| ATOM | 1962 | CB | GLU A 247 | 34.146 | 25.615 | 125.865 | 1.00 | 47.07 |
| ATOM | 1963 | CG | GLU A 247 | 33.161 | 27.569 | 125.185 | 1.00 | 56.16 |
| ATOM | 1964 | CD | GLU A 247 | 31.944 | 26.865 | 124.577 | 1.00 | 62.03 |
| ATOM | 1965 | OE1 | GLU A 247 | 32.096 | 26.088 | 123.607 | 1.00 | 61.85 |
| ATOM | 1966 | OE2 | GLU A 247 | 30.822 | 27.094 | 125.083 | 1.00 | 64.59 |
| ATOM | 1967 | C | GLU A 247 | 34.774 | 24.269 | 125.285 | 1.00 | 39.40 |
| ATOM | 1968 | O | GLU A 247 | 33.727 | 23.879 | 125.794 | 1.00 | 39.91 |
| ATOM | 1969 | N | PRO A 248 | 35.792 | 23.442 | 125.041 | 1.00 | 38.64 |
| ATOM | 1970 | CD | PRO A 248 | 37.101 | 23.817 | 124.483 | 1.00 | 33.25 |
| ATOM | 1971 | CA | PRO A 248 | 35.769 | 22.006 | 125.316 | 1.00 | 35.84 |
| ATOM | 1972 | CB | PRO A 248 | 37.047 | 21.531 | 124.648 | 1.00 | 36.05 |
| ATOM | 1973 | CG | PRO A 248 | 37.970 | 22.687 | 124.982 | 1.00 | 34.21 |
| ATOM | 1974 | C | PRO A 248 | 35.736 | 21.611 | 126.779 | 1.00 | 33.94 |
| ATOM | 1975 | O | PRO A 248 | 36.445 | 22.186 | 127.597 | 1.00 | 32.05 |
| ATOM | 1976 | N | GLU A 249 | 34.914 | 20.616 | 127.096 | 1.00 | 29.39 |
| ATOM | 1977 | CA | GLU A 249 | 34.841 | 20.105 | 128.459 | 1.00 | 33.12 |
| ATOM | 1978 | CB | GLU A 249 | 33.521 | 19.361 | 128.693 | 1.00 | 30.36 |
| ATOM | 1979 | CG | GLU A 249 | 32.284 | 20.212 | 128.564 | 1.00 | 35.98 |
| ATOM | 1980 | CD | GLU A 249 | 31.026 | 19.388 | 128.668 | 1.00 | 40.52 |

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Figure 18-31

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 1981 | OE1 | GLU | A | 249 | 30.817 | 18.509 | 127.804 | 1.00 | 40.27 |
| ATOM | 1982 | OE2 | GLU | A | 249 | 30.252 | 19.609 | 129.620 | 1.00 | 38.57 |
| ATOM | 1983 | C | GLU | A | 249 | 35.995 | 19.119 | 128.623 | 1.00 | 32.30 |
| ATOM | 1984 | O | GLU | A | 249 | 36.472 | 18.884 | 129.728 | 1.00 | 28.51 |
| ATOM | 1985 | N | VAL | A | 250 | 36.434 | 18.547 | 127.502 | 1.00 | 33.74 |
| ATOM | 1986 | CA | VAL | A | 250 | 37.516 | 17.563 | 127.494 | 1.00 | 29.31 |
| ATOM | 1987 | CB | VAL | A | 250 | 36.988 | 16.174 | 127.926 | 1.00 | 29.85 |
| ATOM | 1988 | CG1 | VAL | A | 250 | 35.908 | 15.711 | 126.958 | 1.00 | 24.36 |
| ATOM | 1989 | CG2 | VAL | A | 250 | 38.121 | 15.166 | 127.978 | 1.00 | 25.60 |
| ATOM | 1990 | C | VAL | A | 250 | 38.066 | 17.453 | 126.076 | 1.00 | 29.30 |
| ATOM | 1991 | O | VAL | A | 250 | 37.358 | 17.741 | 125.114 | 1.00 | 24.46 |
| ATOM | 1992 | N | TYR | A | 251 | 39.323 | 17.046 | 125.930 | 1.00 | 27.96 |
| ATOM | 1993 | CA | TYR | A | 251 | 39.865 | 16.913 | 124.585 | 1.00 | 30.06 |
| ATOM | 1994 | CB | TYR | A | 251 | 40.585 | 18.206 | 124.165 | 1.00 | 25.89 |
| ATOM | 1995 | CG | TYR | A | 251 | 41.998 | 18.370 | 124.692 | 1.00 | 29.90 |
| ATOM | 1996 | CD1 | TYR | A | 251 | 43.087 | 17.794 | 124.029 | 1.00 | 26.02 |
| ATOM | 1997 | CE1 | TYR | A | 251 | 44.390 | 17.953 | 124.507 | 1.00 | 29.20 |
| ATOM | 1998 | CD2 | TYR | A | 251 | 42.249 | 19.107 | 125.849 | 1.00 | 31.96 |
| ATOM | 1999 | CE2 | TYR | A | 251 | 43.551 | 19.271 | 126.338 | 1.00 | 31.54 |
| ATOM | 2000 | CZ | TYR | A | 251 | 44.614 | 18.694 | 125.664 | 1.00 | 31.46 |
| ATOM | 2001 | OH | TYR | A | 251 | 45.894 | 18.854 | 126.152 | 1.00 | 29.69 |
| ATOM | 2002 | C | TYR | A | 251 | 40.801 | 15.731 | 124.451 | 1.00 | 27.56 |
| ATOM | 2003 | O | TYR | A | 251 | 41.382 | 15.273 | 125.436 | 1.00 | 28.23 |
| ATOM | 2004 | N | LEU | A | 252 | 40.908 | 15.222 | 123.227 | 1.00 | 23.52 |
| ATOM | 2005 | CA | LEU | A | 252 | 41.806 | 14.117 | 122.919 | 1.00 | 26.53 |
| ATOM | 2006 | CB | LEU | A | 252 | 41.057 | 12.930 | 122.293 | 1.00 | 25.74 |
| ATOM | 2007 | CG | LEU | A | 252 | 40.266 | 12.001 | 123.221 | 1.00 | 28.49 |
| ATOM | 2008 | CD1 | LEU | A | 252 | 39.122 | 12.753 | 123.868 | 1.00 | 27.67 |
| ATOM | 2009 | CD2 | LEU | A | 252 | 39.727 | 10.835 | 122.414 | 1.00 | 32.00 |
| ATOM | 2010 | C | LEU | A | 252 | 42.842 | 14.638 | 121.932 | 1.00 | 27.53 |
| ATOM | 2011 | O | LEU | A | 252 | 42.528 | 15.444 | 121.055 | 1.00 | 24.42 |
| ATOM | 2012 | N | LEU | A | 253 | 44.075 | 14.176 | 122.078 | 1.00 | 24.60 |
| ATOM | 2013 | CA | LEU | A | 253 | 45.157 | 14.599 | 121.204 | 1.00 | 25.04 |
| ATOM | 2014 | CB | LEU | A | 253 | 46.176 | 15.400 | 122.017 | 1.00 | 22.48 |
| ATOM | 2015 | CG | LEU | A | 253 | 47.456 | 15.880 | 121.323 | 1.00 | 21.05 |
| ATOM | 2016 | CD1 | LEU | A | 253 | 47.105 | 16.833 | 120.175 | 1.00 | 23.05 |
| ATOM | 2017 | CD2 | LEU | A | 253 | 48.348 | 16.578 | 122.360 | 1.00 | 16.40 |
| ATOM | 2018 | C | LEU | A | 253 | 45.822 | 13.374 | 120.580 | 1.00 | 23.55 |
| ATOM | 2019 | O | LEU | A | 253 | 46.329 | 12.516 | 121.303 | 1.00 | 22.11 |
| ATOM | 2020 | N | GLN | A | 254 | 45.811 | 13.287 | 119.248 | 1.00 | 22.33 |
| ATOM | 2021 | CA | GLN | A | 254 | 46.417 | 12.150 | 118.552 | 1.00 | 19.84 |
| ATOM | 2022 | CB | GLN | A | 254 | 45.542 | 11.731 | 117.348 | 1.00 | 23.09 |
| ATOM | 2023 | CG | GLN | A | 254 | 46.075 | 12.038 | 115.963 | 1.00 | 35.49 |
| ATOM | 2024 | CD | GLN | A | 254 | 47.073 | 11.017 | 115.453 | 1.00 | 31.26 |
| ATOM | 2025 | OE1 | GLN | A | 254 | 46.712 | 9.937 | 114.961 | 1.00 | 33.69 |
| ATOM | 2026 | NE2 | GLN | A | 254 | 48.338 | 11.349 | 115.574 | 1.00 | 31.02 |
| ATOM | 2027 | C | GLN | A | 254 | 47.831 | 12.576 | 118.153 | 1.00 | 22.46 |
| ATOM | 2028 | O | GLN | A | 254 | 48.034 | 13.599 | 117.478 | 1.00 | 17.56 |
| ATOM | 2029 | N | LEU | A | 255 | 48.804 | 11.781 | 118.590 | 1.00 | 17.64 |
| ATOM | 2030 | CA | LEU | A | 255 | 50.213 | 12.079 | 118.383 | 1.00 | 17.04 |
| ATOM | 2031 | CB | LEU | A | 255 | 50.894 | 12.136 | 119.750 | 1.00 | 14.75 |
| ATOM | 2032 | CG | LEU | A | 255 | 50.277 | 13.196 | 120.670 | 1.00 | 25.02 |
| ATOM | 2033 | CD1 | LEU | A | 255 | 50.732 | 12.996 | 122.107 | 1.00 | 21.99 |
| ATOM | 2034 | CD2 | LEU | A | 255 | 50.636 | 14.578 | 120.149 | 1.00 | 18.30 |
| ATOM | 2035 | C | LEU | A | 255 | 51.023 | 11.169 | 117.476 | 1.00 | 21.34 |
| ATOM | 2036 | O | LEU | A | 255 | 52.089 | 10.705 | 117.875 | 1.00 | 18.73 |
| ATOM | 2037 | N | GLY | A | 256 | 50.543 | 10.928 | 116.259 | 1.00 | 22.75 |
| ATOM | 2038 | CA | GLY | A | 256 | 51.291 | 10.093 | 115.330 | 1.00 | 24.09 |
| ATOM | 2039 | C | GLY | A | 256 | 52.660 | 10.721 | 115.126 | 1.00 | 24.27 |
| ATOM | 2040 | O | GLY | A | 256 | 52.805 | 11.945 | 115.134 | 1.00 | 19.15 |
| ATOM | 2041 | N | THR | A | 257 | 53.680 | 9.903 | 114.948 | 1.00 | 24.14 |
| ATOM | 2042 | CA | THR | A | 257 | 55.014 | 10.440 | 114.765 | 1.00 | 21.32 |
| ATOM | 2043 | CB | THR | A | 257 | 56.048 | 9.582 | 115.511 | 1.00 | 17.24 |
| ATOM | 2044 | OG1 | THR | A | 257 | 56.009 | 8.248 | 115.004 | 1.00 | 17.48 |
| ATOM | 2045 | CG2 | THR | A | 257 | 55.728 | 9.532 | 117.016 | 1.00 | 15.73 |
| ATOM | 2046 | C | THR | A | 257 | 55.403 | 10.527 | 113.290 | 1.00 | 22.98 |

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Figure 18-32

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 2047 | O | THR A 257 | 56.517 | 10.941 | 112.974 | 1.00 | 20.39 |
| ATOM | 2048 | N | ASP A 258 | 54.493 | 10.177 | 112.379 | 1.00 | 22.20 |
| ATOM | 2049 | CA | ASP A 258 | 54.863 | 10.229 | 110.961 | 1.00 | 26.56 |
| ATOM | 2050 | CB | ASP A 258 | 53.849 | 9.496 | 110.056 | 1.00 | 25.06 |
| ATOM | 2051 | CG | ASP A 258 | 52.415 | 9.944 | 110.252 | 1.00 | 29.08 |
| ATOM | 2052 | C | ASP A 258 | 55.222 | 11.596 | 110.364 | 1.00 | 27.87 |
| ATOM | 2053 | O | ASP A 258 | 55.756 | 11.661 | 109.254 | 1.00 | 25.61 |
| ATOM | 2054 | OD1 | ASP A 258 | 52.173 | 11.070 | 110.742 | 1.00 | 29.86 |
| ATOM | 2055 | OD2 | ASP A 258 | 51.513 | 9.168 | 109.869 | 1.00 | 33.25 |
| ATOM | 2056 | N | PRO A 259 | 54.884 | 12.710 | 111.045 | 1.00 | 31.06 |
| ATOM | 2057 | CD | PRO A 259 | 54.019 | 12.928 | 112.220 | 1.00 | 28.59 |
| ATOM | 2058 | CA | PRO A 259 | 55.268 | 14.006 | 110.469 | 1.00 | 30.95 |
| ATOM | 2059 | CB | PRO A 259 | 54.447 | 14.993 | 111.296 | 1.00 | 35.06 |
| ATOM | 2060 | CG | PRO A 259 | 54.418 | 14.320 | 112.636 | 1.00 | 35.26 |
| ATOM | 2061 | C | PRO A 259 | 56.790 | 14.268 | 110.583 | 1.00 | 29.06 |
| ATOM | 2062 | O | PRO A 259 | 57.300 | 15.251 | 110.044 | 1.00 | 29.70 |
| ATOM | 2063 | N | LEU A 260 | 57.508 | 13.389 | 111.280 | 1.00 | 22.68 |
| ATOM | 2064 | CA | LEU A 260 | 58.960 | 13.545 | 111.455 | 1.00 | 28.41 |
| ATOM | 2065 | CB | LEU A 260 | 59.461 | 12.576 | 112.533 | 1.00 | 22.47 |
| ATOM | 2066 | CG | LEU A 260 | 58.970 | 12.791 | 113.969 | 1.00 | 20.14 |
| ATOM | 2067 | CD1 | LEU A 260 | 59.352 | 11.599 | 114.826 | 1.00 | 22.83 |
| ATOM | 2068 | CD2 | LEU A 260 | 59.592 | 14.079 | 114.532 | 1.00 | 20.48 |
| ATOM | 2069 | C | LEU A 260 | 59.770 | 13.344 | 110.160 | 1.00 | 27.95 |
| ATOM | 2070 | O | LEU A 260 | 59.407 | 12.535 | 109.299 | 1.00 | 27.03 |
| ATOM | 2071 | N | LEU A 261 | 60.874 | 14.081 | 110.040 | 1.00 | 26.76 |
| ATOM | 2072 | CA | LEU A 261 | 61.742 | 14.010 | 108.865 | 1.00 | 26.56 |
| ATOM | 2073 | CB | LEU A 261 | 63.067 | 14.737 | 109.137 | 1.00 | 23.06 |
| ATOM | 2074 | CG | LEU A 261 | 64.131 | 14.615 | 108.025 | 1.00 | 29.52 |
| ATOM | 2075 | CD1 | LEU A 261 | 63.642 | 15.325 | 106.770 | 1.00 | 22.68 |
| ATOM | 2076 | CD2 | LEU A 261 | 65.460 | 15.219 | 108.475 | 1.00 | 26.71 |
| ATOM | 2077 | C | LEU A 261 | 62.063 | 12.577 | 108.443 | 1.00 | 28.23 |
| ATOM | 2078 | O | LEU A 261 | 61.880 | 12.198 | 107.289 | 1.00 | 26.52 |
| ATOM | 2079 | N | GLU A 262 | 62.539 | 11.787 | 109.397 | 1.00 | 28.70 |
| ATOM | 2080 | CA | GLU A 262 | 62.938 | 10.416 | 109.135 | 1.00 | 31.76 |
| ATOM | 2081 | CB | GLU A 262 | 63.685 | 9.855 | 110.351 | 1.00 | 29.72 |
| ATOM | 2082 | CG | GLU A 262 | 64.890 | 10.683 | 110.803 | 1.00 | 31.33 |
| ATOM | 2083 | CD | GLU A 262 | 64.521 | 11.847 | 111.708 | 1.00 | 28.07 |
| ATOM | 2084 | OE1 | GLU A 262 | 63.324 | 12.195 | 111.789 | 1.00 | 28.75 |
| ATOM | 2085 | OE2 | GLU A 262 | 65.433 | 12.424 | 112.340 | 1.00 | 26.08 |
| ATOM | 2086 | C | GLU A 262 | 61.847 | 9.429 | 108.721 | 1.00 | 28.63 |
| ATOM | 2087 | O | GLU A 262 | 62.158 | 8.305 | 108.350 | 1.00 | 29.72 |
| ATOM | 2088 | N | ASP A 263 | 60.582 | 9.825 | 108.785 | 1.00 | 28.07 |
| ATOM | 2089 | CA | ASP A 263 | 59.513 | 8.902 | 108.412 | 1.00 | 26.85 |
| ATOM | 2090 | CB | ASP A 263 | 58.305 | 9.099 | 109.333 | 1.00 | 25.26 |
| ATOM | 2091 | CG | ASP A 263 | 57.261 | 7.998 | 109.185 | 1.00 | 33.14 |
| ATOM | 2092 | OD1 | ASP A 263 | 56.638 | 7.636 | 110.209 | 1.00 | 29.91 |
| ATOM | 2093 | OD2 | ASP A 263 | 57.042 | 7.509 | 108.051 | 1.00 | 26.56 |
| ATOM | 2094 | C | ASP A 263 | 59.150 | 9.146 | 106.957 | 1.00 | 29.44 |
| ATOM | 2095 | O | ASP A 263 | 58.740 | 10.247 | 106.594 | 1.00 | 24.70 |
| ATOM | 2096 | N | TYR A 264 | 59.303 | 8.111 | 106.130 | 1.00 | 27.51 |
| ATOM | 2097 | CA | TYR A 264 | 59.031 | 8.219 | 104.696 | 1.00 | 33.89 |
| ATOM | 2098 | CB | TYR A 264 | 59.576 | 7.008 | 103.935 | 1.00 | 40.44 |
| ATOM | 2099 | CG | TYR A 264 | 61.059 | 6.771 | 104.092 | 1.00 | 50.64 |
| ATOM | 2100 | CD1 | TYR A 264 | 61.565 | 6.087 | 105.199 | 1.00 | 54.67 |
| ATOM | 2101 | CE1 | TYR A 264 | 62.933 | 5.876 | 105.351 | 1.00 | 55.28 |
| ATOM | 2102 | CD2 | TYR A 264 | 61.960 | 7.242 | 103.140 | 1.00 | 53.79 |
| ATOM | 2103 | CE2 | TYR A 264 | 63.329 | 7.038 | 103.282 | 1.00 | 56.61 |
| ATOM | 2104 | CZ | TYR A 264 | 63.809 | 6.354 | 104.388 | 1.00 | 56.22 |
| ATOM | 2105 | OH | TYR A 264 | 65.161 | 6.147 | 104.524 | 1.00 | 55.90 |
| ATOM | 2106 | C | TYR A 264 | 57.581 | 8.394 | 104.294 | 1.00 | 31.33 |
| ATOM | 2107 | O | TYR A 264 | 57.311 | 8.825 | 103.178 | 1.00 | 27.15 |
| ATOM | 2108 | N | LEU A 265 | 56.641 | 8.059 | 105.172 | 1.00 | 26.88 |
| ATOM | 2109 | CA | LEU A 265 | 55.244 | 8.209 | 104.792 | 1.00 | 24.39 |
| ATOM | 2110 | CB | LEU A 265 | 54.360 | 7.189 | 105.527 | 1.00 | 26.55 |
| ATOM | 2111 | CG | LEU A 265 | 54.663 | 5.724 | 105.168 | 1.00 | 29.80 |
| ATOM | 2112 | CD1 | LEU A 265 | 53.464 | 4.836 | 105.503 | 1.00 | 21.17 |

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Figure 18-33

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 2113 | CD2 | LEU | A | 265 | 54.931 | 5.620 | 103.682 | 1.00 | 33.35 |
| ATOM | 2114 | C | LEU | A | 265 | 54.669 | 9.617 | 104.921 | 1.00 | 20.81 |
| ATOM | 2115 | O | LEU | A | 265 | 53.457 | 9.796 | 104.979 | 1.00 | 21.30 |
| ATOM | 2116 | N | SER | A | 266 | 55.540 | 10.622 | 104.959 | 1.00 | 23.23 |
| ATOM | 2117 | CA | SER | A | 266 | 55.084 | 12.011 | 105.008 | 1.00 | 26.30 |
| ATOM | 2118 | CB | SER | A | 266 | 54.856 | 12.502 | 106.444 | 1.00 | 25.16 |
| ATOM | 2119 | OG | SER | A | 266 | 56.074 | 12.845 | 107.084 | 1.00 | 22.92 |
| ATOM | 2120 | C | SER | A | 266 | 56.147 | 12.879 | 104.355 | 1.00 | 30.17 |
| ATOM | 2121 | O | SER | A | 266 | 57.334 | 12.555 | 104.385 | 1.00 | 31.65 |
| ATOM | 2122 | N | LYS | A | 267 | 55.731 | 13.985 | 103.757 | 1.00 | 31.56 |
| ATOM | 2123 | CA | LYS | A | 267 | 56.696 | 14.873 | 103.140 | 1.00 | 27.65 |
| ATOM | 2124 | CB | LYS | A | 267 | 56.140 | 15.425 | 101.834 | 1.00 | 30.54 |
| ATOM | 2125 | CG | LYS | A | 267 | 55.815 | 14.327 | 100.819 | 1.00 | 34.13 |
| ATOM | 2126 | CD | LYS | A | 267 | 57.039 | 13.463 | 100.549 | 1.00 | 29.09 |
| ATOM | 2127 | CE | LYS | A | 267 | 56.745 | 12.376 | 99.524 | 1.00 | 37.61 |
| ATOM | 2128 | NZ | LYS | A | 267 | 57.956 | 11.541 | 99.272 | 1.00 | 31.91 |
| ATOM | 2129 | C | LYS | A | 267 | 57.050 | 16.004 | 104.107 | 1.00 | 30.85 |
| ATOM | 2130 | O | LYS | A | 267 | 57.624 | 17.017 | 103.707 | 1.00 | 27.86 |
| ATOM | 2131 | N | PHE | A | 268 | 56.688 | 15.826 | 105.377 | 1.00 | 24.19 |
| ATOM | 2132 | CA | PHE | A | 268 | 57.009 | 16.808 | 106.412 | 1.00 | 25.34 |
| ATOM | 2133 | CB | PHE | A | 268 | 56.014 | 16.730 | 107.579 | 1.00 | 24.54 |
| ATOM | 2134 | CG | PHE | A | 268 | 54.636 | 17.256 | 107.257 | 1.00 | 21.68 |
| ATOM | 2135 | CD1 | PHE | A | 268 | 53.631 | 17.221 | 108.216 | 1.00 | 28.65 |
| ATOM | 2136 | CD2 | PHE | A | 268 | 54.346 | 17.806 | 106.011 | 1.00 | 25.14 |
| ATOM | 2137 | CE1 | PHE | A | 268 | 52.357 | 17.728 | 107.944 | 1.00 | 25.34 |
| ATOM | 2138 | CE2 | PHE | A | 268 | 53.077 | 18.315 | 105.730 | 1.00 | 23.79 |
| ATOM | 2139 | CZ | PHE | A | 268 | 52.082 | 18.275 | 106.702 | 1.00 | 28.13 |
| ATOM | 2140 | C | PHE | A | 268 | 58.410 | 16.470 | 106.908 | 1.00 | 25.66 |
| ATOM | 2141 | O | PHE | A | 268 | 58.778 | 15.299 | 106.994 | 1.00 | 28.44 |
| ATOM | 2142 | N | ASN | A | 269 | 59.194 | 17.490 | 107.230 | 1.00 | 25.81 |
| ATOM | 2143 | CA | ASN | A | 269 | 60.555 | 17.270 | 107.709 | 1.00 | 30.60 |
| ATOM | 2144 | CB | ASN | A | 269 | 61.566 | 17.938 | 106.767 | 1.00 | 31.97 |
| ATOM | 2145 | CG | ASN | A | 269 | 61.392 | 17.513 | 105.317 | 1.00 | 35.83 |
| ATOM | 2146 | OD1 | ASN | A | 269 | 61.235 | 16.332 | 105.020 | 1.00 | 33.93 |
| ATOM | 2147 | ND2 | ASN | A | 269 | 61.446 | 18.477 | 104.405 | 1.00 | 33.95 |
| ATOM | 2148 | C | ASN | A | 269 | 60.723 | 17.843 | 109.110 | 1.00 | 31.80 |
| ATOM | 2149 | O | ASN | A | 269 | 61.609 | 18.665 | 109.348 | 1.00 | 28.13 |
| ATOM | 2150 | N | LEU | A | 270 | 59.888 | 17.397 | 110.043 | 1.00 | 29.70 |
| ATOM | 2151 | CA | LEU | A | 270 | 59.954 | 17.918 | 111.406 | 1.00 | 26.87 |
| ATOM | 2152 | CB | LEU | A | 270 | 58.575 | 17.833 | 112.074 | 1.00 | 26.60 |
| ATOM | 2153 | CG | LEU | A | 270 | 57.392 | 18.425 | 111.297 | 1.00 | 29.62 |
| ATOM | 2154 | CD1 | LEU | A | 270 | 56.177 | 18.494 | 112.222 | 1.00 | 28.54 |
| ATOM | 2155 | CD2 | LEU | A | 270 | 57.740 | 19.825 | 110.790 | 1.00 | 29.40 |
| ATOM | 2156 | C | LEU | A | 270 | 60.979 | 17.242 | 112.301 | 1.00 | 26.83 |
| ATOM | 2157 | O | LEU | A | 270 | 61.490 | 16.158 | 111.990 | 1.00 | 19.60 |
| ATOM | 2158 | N | SER | A | 271 | 61.275 | 17.896 | 113.420 | 1.00 | 21.66 |
| ATOM | 2159 | CA | SER | A | 271 | 62.220 | 17.365 | 114.393 | 1.00 | 27.08 |
| ATOM | 2160 | CB | SER | A | 271 | 63.189 | 18.460 | 114.846 | 1.00 | 24.64 |
| ATOM | 2161 | OG | SER | A | 271 | 62.499 | 19.433 | 115.626 | 1.00 | 18.60 |
| ATOM | 2162 | C | SER | A | 271 | 61.454 | 16.868 | 115.618 | 1.00 | 23.70 |
| ATOM | 2163 | O | SER | A | 271 | 60.272 | 17.150 | 115.772 | 1.00 | 22.56 |
| ATOM | 2164 | N | ASN | A | 272 | 62.157 | 16.129 | 116.470 | 1.00 | 28.35 |
| ATOM | 2165 | CA | ASN | A | 272 | 61.649 | 15.593 | 117.739 | 1.00 | 31.03 |
| ATOM | 2166 | CB | ASN | A | 272 | 62.774 | 14.880 | 118.498 | 1.00 | 28.80 |
| ATOM | 2167 | CG | ASN | A | 272 | 62.854 | 13.428 | 118.180 | 1.00 | 36.65 |
| ATOM | 2168 | OD1 | ASN | A | 272 | 63.712 | 12.709 | 118.705 | 1.00 | 29.89 |
| ATOM | 2169 | ND2 | ASN | A | 272 | 61.953 | 12.969 | 117.319 | 1.00 | 40.80 |
| ATOM | 2170 | C | ASN | A | 272 | 61.167 | 16.695 | 118.661 | 1.00 | 31.83 |
| ATOM | 2171 | O | ASN | A | 272 | 60.090 | 16.618 | 119.261 | 1.00 | 27.50 |
| ATOM | 2172 | N | VAL | A | 273 | 62.032 | 17.693 | 118.804 | 1.00 | 31.49 |
| ATOM | 2173 | CA | VAL | A | 273 | 61.802 | 18.837 | 119.667 | 1.00 | 31.58 |
| ATOM | 2174 | CB | VAL | A | 273 | 63.069 | 19.709 | 119.725 | 1.00 | 35.80 |
| ATOM | 2175 | CG1 | VAL | A | 273 | 62.804 | 20.988 | 120.500 | 1.00 | 48.07 |
| ATOM | 2176 | CG2 | VAL | A | 273 | 64.198 | 18.914 | 120.381 | 1.00 | 42.81 |
| ATOM | 2177 | C | VAL | A | 273 | 60.608 | 19.665 | 119.234 | 1.00 | 30.13 |
| ATOM | 2178 | O | VAL | A | 273 | 59.872 | 20.174 | 120.072 | 1.00 | 31.44 |

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Figure 18-34

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 2179 | N | ALA | A | 274 | 60.405 | 19.800 | 117.929 | 1.00 | 24.15 |
| ATOM | 2180 | CA | ALA | A | 274 | 59.258 | 20.558 | 117.455 | 1.00 | 26.27 |
| ATOM | 2181 | CB | ALA | A | 274 | 59.341 | 20.780 | 115.965 | 1.00 | 21.85 |
| ATOM | 2182 | C | ALA | A | 274 | 58.005 | 19.759 | 117.789 | 1.00 | 25.68 |
| ATOM | 2183 | O | ALA | A | 274 | 56.961 | 20.324 | 118.132 | 1.00 | 23.76 |
| ATOM | 2184 | N | PHE | A | 275 | 58.122 | 18.438 | 117.680 | 1.00 | 25.20 |
| ATOM | 2185 | CA | PHE | A | 275 | 57.015 | 17.538 | 117.974 | 1.00 | 25.89 |
| ATOM | 2186 | CB | PHE | A | 275 | 57.449 | 16.092 | 117.710 | 1.00 | 25.21 |
| ATOM | 2187 | CG | PHE | A | 275 | 56.340 | 15.088 | 117.870 | 1.00 | 28.85 |
| ATOM | 2188 | CD1 | PHE | A | 275 | 55.278 | 15.064 | 116.982 | 1.00 | 32.60 |
| ATOM | 2189 | CD2 | PHE | A | 275 | 56.365 | 14.166 | 118.910 | 1.00 | 28.93 |
| ATOM | 2190 | CE1 | PHE | A | 275 | 54.248 | 14.132 | 117.119 | 1.00 | 33.75 |
| ATOM | 2191 | CE2 | PHE | A | 275 | 55.343 | 13.231 | 119.059 | 1.00 | 30.83 |
| ATOM | 2192 | CZ | PHE | A | 275 | 54.282 | 13.214 | 118.160 | 1.00 | 34.19 |
| ATOM | 2193 | C | PHE | A | 275 | 56.607 | 17.712 | 119.445 | 1.00 | 24.63 |
| ATOM | 2194 | O | PHE | A | 275 | 55.428 | 17.877 | 119.767 | 1.00 | 22.40 |
| ATOM | 2195 | N | LEU | A | 276 | 57.594 | 17.673 | 120.331 | 1.00 | 25.45 |
| ATOM | 2196 | CA | LEU | A | 276 | 57.357 | 17.837 | 121.766 | 1.00 | 27.94 |
| ATOM | 2197 | CB | LEU | A | 276 | 58.667 | 17.692 | 122.534 | 1.00 | 26.11 |
| ATOM | 2198 | CG | LEU | A | 276 | 58.651 | 18.132 | 124.001 | 1.00 | 31.15 |
| ATOM | 2199 | CD1 | LEU | A | 276 | 57.609 | 17.351 | 124.761 | 1.00 | 29.37 |
| ATOM | 2200 | CD2 | LEU | A | 276 | 60.033 | 17.937 | 124.612 | 1.00 | 27.98 |
| ATOM | 2201 | C | LEU | A | 276 | 56.770 | 19.208 | 122.058 | 1.00 | 30.12 |
| ATOM | 2202 | O | LEU | A | 276 | 55.822 | 19.348 | 122.838 | 1.00 | 28.69 |
| ATOM | 2203 | N | LYS | A | 277 | 57.353 | 20.219 | 121.425 | 1.00 | 30.99 |
| ATOM | 2204 | CA | LYS | A | 277 | 56.913 | 21.593 | 121.603 | 1.00 | 27.04 |
| ATOM | 2205 | CB | LYS | A | 277 | 57.742 | 22.516 | 120.704 | 1.00 | 30.38 |
| ATOM | 2206 | CG | LYS | A | 277 | 57.941 | 23.934 | 121.237 | 1.00 | 36.46 |
| ATOM | 2207 | CD | LYS | A | 277 | 56.633 | 24.668 | 121.454 | 1.00 | 42.73 |
| ATOM | 2208 | CE | LYS | A | 277 | 56.870 | 26.059 | 122.049 | 1.00 | 45.70 |
| ATOM | 2209 | NZ | LYS | A | 277 | 57.528 | 26.004 | 123.390 | 1.00 | 44.64 |
| ATOM | 2210 | C | LYS | A | 277 | 55.432 | 21.683 | 121.242 | 1.00 | 30.26 |
| ATOM | 2211 | O | LYS | A | 277 | 54.640 | 22.284 | 121.972 | 1.00 | 27.55 |
| ATOM | 2212 | N | ALA | A | 278 | 55.057 | 21.078 | 120.115 | 1.00 | 30.15 |
| ATOM | 2213 | CA | ALA | A | 278 | 53.662 | 21.096 | 119.676 | 1.00 | 30.51 |
| ATOM | 2214 | CB | ALA | A | 278 | 53.496 | 20.270 | 118.406 | 1.00 | 28.96 |
| ATOM | 2215 | C | ALA | A | 278 | 52.789 | 20.527 | 120.786 | 1.00 | 30.99 |
| ATOM | 2216 | O | ALA | A | 278 | 51.735 | 21.067 | 121.108 | 1.00 | 30.36 |
| ATOM | 2217 | N | PHE | A | 279 | 53.245 | 19.422 | 121.360 | 1.00 | 27.85 |
| ATOM | 2218 | CA | PHE | A | 279 | 52.540 | 18.759 | 122.448 | 1.00 | 29.62 |
| ATOM | 2219 | CB | PHE | A | 279 | 53.343 | 17.534 | 122.886 | 1.00 | 26.83 |
| ATOM | 2220 | CG | PHE | A | 279 | 52.786 | 16.823 | 124.078 | 1.00 | 29.11 |
| ATOM | 2221 | CD1 | PHE | A | 279 | 51.556 | 16.176 | 124.015 | 1.00 | 28.86 |
| ATOM | 2222 | CD2 | PHE | A | 279 | 53.505 | 16.786 | 125.267 | 1.00 | 33.03 |
| ATOM | 2223 | CE1 | PHE | A | 279 | 51.054 | 15.500 | 125.121 | 1.00 | 37.90 |
| ATOM | 2224 | CE2 | PHE | A | 279 | 53.011 | 16.114 | 126.386 | 1.00 | 38.01 |
| ATOM | 2225 | CZ | PHE | A | 279 | 51.783 | 15.469 | 126.313 | 1.00 | 36.11 |
| ATOM | 2226 | C | PHE | A | 279 | 52.362 | 19.730 | 123.621 | 1.00 | 30.97 |
| ATOM | 2227 | O | PHE | A | 279 | 51.265 | 19.853 | 124.184 | 1.00 | 26.26 |
| ATOM | 2228 | N | ASN | A | 280 | 53.432 | 20.429 | 123.990 | 1.00 | 32.03 |
| ATOM | 2229 | CA | ASN | A | 280 | 53.339 | 21.373 | 125.104 | 1.00 | 30.54 |
| ATOM | 2230 | CB | ASN | A | 280 | 54.724 | 21.819 | 125.583 | 1.00 | 26.79 |
| ATOM | 2231 | CG | ASN | A | 280 | 55.508 | 20.695 | 126.227 | 1.00 | 33.66 |
| ATOM | 2232 | OD1 | ASN | A | 280 | 54.958 | 19.886 | 126.971 | 1.00 | 34.47 |
| ATOM | 2233 | ND2 | ASN | A | 280 | 56.809 | 20.660 | 125.973 | 1.00 | 33.59 |
| ATOM | 2234 | C | ASN | A | 280 | 52.493 | 22.587 | 124.781 | 1.00 | 30.46 |
| ATOM | 2235 | O | ASN | A | 280 | 51.899 | 23.182 | 125.677 | 1.00 | 27.66 |
| ATOM | 2236 | N | ILE | A | 281 | 52.429 | 22.960 | 123.509 | 1.00 | 27.32 |
| ATOM | 2237 | CA | ILE | A | 281 | 51.620 | 24.107 | 123.128 | 1.00 | 31.07 |
| ATOM | 2238 | CB | ILE | A | 281 | 51.878 | 24.517 | 121.666 | 1.00 | 35.08 |
| ATOM | 2239 | CG2 | ILE | A | 281 | 50.776 | 25.445 | 121.174 | 1.00 | 34.33 |
| ATOM | 2240 | CG1 | ILE | A | 281 | 53.253 | 25.185 | 121.562 | 1.00 | 33.53 |
| ATOM | 2241 | CD1 | ILE | A | 281 | 53.590 | 25.694 | 120.178 | 1.00 | 34.88 |
| ATOM | 2242 | C | ILE | A | 281 | 50.141 | 23.798 | 123.329 | 1.00 | 31.22 |
| ATOM | 2243 | O | ILE | A | 281 | 49.391 | 24.621 | 123.854 | 1.00 | 30.15 |
| ATOM | 2244 | N | VAL | A | 282 | 49.723 | 22.606 | 122.923 | 1.00 | 30.91 |

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Figure 18-35

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 2245 | CA | VAL | A | 282 | 48.332 | 22.214 | 123.081 | 1.00 | 30.76 |
| ATOM | 2246 | CB | VAL | A | 282 | 48.075 | 20.797 | 122.523 | 1.00 | 35.10 |
| ATOM | 2247 | CG1 | VAL | A | 282 | 46.641 | 20.358 | 122.841 | 1.00 | 28.72 |
| ATOM | 2248 | CG2 | VAL | A | 282 | 48.313 | 20.781 | 121.018 | 1.00 | 28.66 |
| ATOM | 2249 | C | VAL | A | 282 | 47.952 | 22.236 | 124.558 | 1.00 | 31.39 |
| ATOM | 2250 | O | VAL | A | 282 | 46.884 | 22.715 | 124.917 | 1.00 | 32.70 |
| ATOM | 2251 | N | ARG | A | 283 | 48.837 | 21.720 | 125.406 | 1.00 | 29.86 |
| ATOM | 2252 | CA | ARG | A | 283 | 48.587 | 21.675 | 126.840 | 1.00 | 34.82 |
| ATOM | 2253 | CB | ARG | A | 283 | 49.629 | 20.785 | 127.519 | 1.00 | 31.44 |
| ATOM | 2254 | CG | ARG | A | 283 | 49.551 | 19.334 | 127.061 | 1.00 | 29.49 |
| ATOM | 2255 | CD | ARG | A | 283 | 50.729 | 18.539 | 127.554 | 1.00 | 30.67 |
| ATOM | 2256 | NE | ARG | A | 283 | 50.730 | 18.314 | 128.990 | 1.00 | 30.78 |
| ATOM | 2257 | CZ | ARG | A | 283 | 51.826 | 18.351 | 129.742 | 1.00 | 35.27 |
| ATOM | 2258 | NH1 | ARG | A | 283 | 53.012 | 18.611 | 129.198 | 1.00 | 36.46 |
| ATOM | 2259 | NH2 | ARG | A | 283 | 51.742 | 18.100 | 131.035 | 1.00 | 35.90 |
| ATOM | 2260 | C | ARG | A | 283 | 48.561 | 23.065 | 127.473 | 1.00 | 36.06 |
| ATOM | 2261 | O | ARG | A | 283 | 47.830 | 23.302 | 128.439 | 1.00 | 35.04 |
| ATOM | 2262 | N | GLU | A | 284 | 49.350 | 23.985 | 126.928 | 1.00 | 35.70 |
| ATOM | 2263 | CA | GLU | A | 284 | 49.376 | 25.348 | 127.448 | 1.00 | 40.93 |
| ATOM | 2264 | CB | GLU | A | 284 | 50.499 | 26.166 | 126.799 | 1.00 | 44.17 |
| ATOM | 2265 | CG | GLU | A | 284 | 51.917 | 25.702 | 127.141 | 1.00 | 56.39 |
| ATOM | 2266 | CD | GLU | A | 284 | 52.989 | 26.495 | 126.401 | 1.00 | 60.69 |
| ATOM | 2267 | OE1 | GLU | A | 284 | 53.012 | 27.738 | 126.542 | 1.00 | 63.13 |
| ATOM | 2268 | OE2 | GLU | A | 284 | 53.810 | 25.880 | 125.680 | 1.00 | 62.79 |
| ATOM | 2269 | C | GLU | A | 284 | 48.039 | 26.014 | 127.148 | 1.00 | 39.24 |
| ATOM | 2270 | O | GLU | A | 284 | 47.525 | 26.783 | 127.954 | 1.00 | 38.52 |
| ATOM | 2271 | N | VAL | A | 285 | 47.472 | 25.704 | 125.986 | 1.00 | 33.75 |
| ATOM | 2272 | CA | VAL | A | 285 | 46.205 | 26.294 | 125.592 | 1.00 | 35.82 |
| ATOM | 2273 | CB | VAL | A | 285 | 46.039 | 26.291 | 124.062 | 1.00 | 34.14 |
| ATOM | 2274 | CG1 | VAL | A | 285 | 44.654 | 26.811 | 123.693 | 1.00 | 36.43 |
| ATOM | 2275 | CG2 | VAL | A | 285 | 47.114 | 27.153 | 123.419 | 1.00 | 37.26 |
| ATOM | 2276 | C | VAL | A | 285 | 44.964 | 25.638 | 126.192 | 1.00 | 38.96 |
| ATOM | 2277 | O | VAL | A | 285 | 44.043 | 26.336 | 126.611 | 1.00 | 41.83 |
| ATOM | 2278 | N | PHE | A | 286 | 44.931 | 24.308 | 126.236 | 1.00 | 37.57 |
| ATOM | 2279 | CA | PHE | A | 286 | 43.760 | 23.608 | 126.753 | 1.00 | 35.05 |
| ATOM | 2280 | CB | PHE | A | 286 | 43.159 | 22.723 | 125.657 | 1.00 | 32.53 |
| ATOM | 2281 | CG | PHE | A | 286 | 42.544 | 23.490 | 124.529 | 1.00 | 30.15 |
| ATOM | 2282 | CD1 | PHE | A | 286 | 43.104 | 23.459 | 123.256 | 1.00 | 33.96 |
| ATOM | 2283 | CD2 | PHE | A | 286 | 41.398 | 24.245 | 124.736 | 1.00 | 30.30 |
| ATOM | 2284 | CE1 | PHE | A | 286 | 42.527 | 24.170 | 122.202 | 1.00 | 32.96 |
| ATOM | 2285 | CE2 | PHE | A | 286 | 40.813 | 24.958 | 123.693 | 1.00 | 31.67 |
| ATOM | 2286 | CZ | PHE | A | 286 | 41.381 | 24.919 | 122.419 | 1.00 | 31.66 |
| ATOM | 2287 | C | PHE | A | 286 | 43.922 | 22.773 | 128.015 | 1.00 | 35.18 |
| ATOM | 2288 | O | PHE | A | 286 | 42.984 | 22.080 | 128.409 | 1.00 | 36.97 |
| ATOM | 2289 | N | GLY | A | 287 | 45.086 | 22.840 | 128.656 | 1.00 | 30.87 |
| ATOM | 2290 | CA | GLY | A | 287 | 45.297 | 22.056 | 129.862 | 1.00 | 30.06 |
| ATOM | 2291 | C | GLY | A | 287 | 45.525 | 20.590 | 129.527 | 1.00 | 34.44 |
| ATOM | 2292 | O | GLY | A | 287 | 45.914 | 20.264 | 128.403 | 1.00 | 32.54 |
| ATOM | 2293 | N | GLU | A | 288 | 45.288 | 19.710 | 130.500 | 1.00 | 28.42 |
| ATOM | 2294 | CA | GLU | A | 288 | 45.464 | 18.273 | 130.310 | 1.00 | 32.23 |
| ATOM | 2295 | CB | GLU | A | 288 | 45.613 | 17.576 | 131.663 | 1.00 | 37.02 |
| ATOM | 2296 | CG | GLU | A | 288 | 46.910 | 17.864 | 132.411 | 1.00 | 45.36 |
| ATOM | 2297 | CD | GLU | A | 288 | 48.140 | 17.455 | 131.622 | 1.00 | 45.65 |
| ATOM | 2298 | OE1 | GLU | A | 288 | 48.144 | 16.334 | 131.069 | 1.00 | 46.42 |
| ATOM | 2299 | OE2 | GLU | A | 288 | 49.106 | 18.245 | 131.571 | 1.00 | 50.78 |
| ATOM | 2300 | C | GLU | A | 288 | 44.309 | 17.623 | 129.546 | 1.00 | 30.98 |
| ATOM | 2301 | O | GLU | A | 288 | 43.144 | 17.957 | 129.762 | 1.00 | 28.67 |
| ATOM | 2302 | N | GLY | A | 289 | 44.641 | 16.694 | 128.657 | 1.00 | 29.66 |
| ATOM | 2303 | CA | GLY | A | 289 | 43.625 | 15.999 | 127.886 | 1.00 | 28.08 |
| ATOM | 2304 | C | GLY | A | 289 | 43.922 | 14.510 | 127.861 | 1.00 | 30.45 |
| ATOM | 2305 | O | GLY | A | 289 | 44.618 | 14.307 | 128.739 | 1.00 | 25.90 |
| ATOM | 2306 | N | VAL | A | 290 | 43.384 | 13.807 | 126.868 | 1.00 | 26.21 |
| ATOM | 2307 | CA | VAL | A | 290 | 43.612 | 12.373 | 126.718 | 1.00 | 27.31 |
| ATOM | 2308 | CB | VAL | A | 290 | 42.288 | 11.626 | 126.412 | 1.00 | 26.53 |
| ATOM | 2309 | CG1 | VAL | A | 290 | 42.554 | 10.148 | 126.204 | 1.00 | 25.36 |
| ATOM | 2310 | CG2 | VAL | A | 290 | 41.308 | 11.822 | 127.565 | 1.00 | 24.38 |

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Figure 18-36

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 2311 | C | VAL | A | 290 | 44.580 | 12.248 | 125.550 | 1.00 | 24.52 |
| ATOM | 2312 | O | VAL | A | 290 | 44.307 | 12.743 | 124.461 | 1.00 | 26.84 |
| ATOM | 2313 | N | TYR | A | 291 | 45.716 | 11.597 | 125.775 | 1.00 | 23.56 |
| ATOM | 2314 | CA | TYR | A | 291 | 46.729 | 11.478 | 124.732 | 1.00 | 23.74 |
| ATOM | 2315 | CB | TYR | A | 291 | 48.092 | 11.817 | 125.342 | 1.00 | 18.40 |
| ATOM | 2316 | CG | TYR | A | 291 | 48.040 | 13.113 | 126.118 | 1.00 | 21.60 |
| ATOM | 2317 | CD1 | TYR | A | 291 | 48.326 | 13.148 | 127.483 | 1.00 | 23.83 |
| ATOM | 2318 | CE1 | TYR | A | 291 | 48.200 | 14.331 | 128.214 | 1.00 | 24.57 |
| ATOM | 2319 | CD2 | TYR | A | 291 | 47.634 | 14.291 | 125.503 | 1.00 | 18.17 |
| ATOM | 2320 | CE2 | TYR | A | 291 | 47.504 | 15.476 | 126.220 | 1.00 | 26.36 |
| ATOM | 2321 | CZ | TYR | A | 291 | 47.786 | 15.489 | 127.575 | 1.00 | 27.68 |
| ATOM | 2322 | OH | TYR | A | 291 | 47.631 | 16.657 | 128.283 | 1.00 | 28.92 |
| ATOM | 2323 | C | TYR | A | 291 | 46.768 | 10.118 | 124.044 | 1.00 | 23.03 |
| ATOM | 2324 | O | TYR | A | 291 | 46.837 | 9.082 | 124.707 | 1.00 | 20.66 |
| ATOM | 2325 | N | LEU | A | 292 | 46.755 | 10.142 | 122.711 | 1.00 | 23.96 |
| ATOM | 2326 | CA | LEU | A | 292 | 46.767 | 8.924 | 121.902 | 1.00 | 20.69 |
| ATOM | 2327 | CB | LEU | A | 292 | 45.482 | 8.842 | 121.076 | 1.00 | 22.13 |
| ATOM | 2328 | CG | LEU | A | 292 | 44.162 | 9.063 | 121.814 | 1.00 | 23.78 |
| ATOM | 2329 | CD1 | LEU | A | 292 | 43.001 | 8.959 | 120.826 | 1.00 | 23.09 |
| ATOM | 2330 | CD2 | LEU | A | 292 | 44.008 | 8.050 | 122.930 | 1.00 | 16.01 |
| ATOM | 2331 | C | LEU | A | 292 | 47.953 | 8.885 | 120.947 | 1.00 | 22.90 |
| ATOM | 2332 | O | LEU | A | 292 | 48.527 | 9.923 | 120.617 | 1.00 | 22.31 |
| ATOM | 2333 | N | GLY | A | 293 | 48.301 | 7.684 | 120.491 | 1.00 | 18.83 |
| ATOM | 2334 | CA | GLY | A | 293 | 49.401 | 7.529 | 119.554 | 1.00 | 24.35 |
| ATOM | 2335 | C | GLY | A | 293 | 48.908 | 7.846 | 118.154 | 1.00 | 24.22 |
| ATOM | 2336 | O | GLY | A | 293 | 48.025 | 8.684 | 117.991 | 1.00 | 20.46 |
| ATOM | 2337 | N | GLY | A | 294 | 49.459 | 7.177 | 117.148 | 1.00 | 24.63 |
| ATOM | 2338 | CA | GLY | A | 294 | 49.035 | 7.423 | 115.779 | 1.00 | 22.03 |
| ATOM | 2339 | C | GLY | A | 294 | 50.024 | 6.869 | 114.769 | 1.00 | 22.90 |
| ATOM | 2340 | O | GLY | A | 294 | 50.956 | 6.150 | 115.136 | 1.00 | 24.10 |
| ATOM | 2341 | N | GLY | A | 295 | 49.825 | 7.203 | 113.499 | 1.00 | 19.85 |
| ATOM | 2342 | CA | GLY | A | 295 | 50.721 | 6.724 | 112.458 | 1.00 | 23.33 |
| ATOM | 2343 | C | GLY | A | 295 | 52.185 | 7.010 | 112.740 | 1.00 | 19.01 |
| ATOM | 2344 | O | GLY | A | 295 | 52.541 | 8.094 | 113.196 | 1.00 | 19.39 |
| ATOM | 2345 | N | GLY | A | 296 | 53.035 | 6.026 | 112.472 | 1.00 | 25.85 |
| ATOM | 2346 | CA | GLY | A | 296 | 54.468 | 6.162 | 112.690 | 1.00 | 22.65 |
| ATOM | 2347 | C | GLY | A | 296 | 55.098 | 4.898 | 112.146 | 1.00 | 25.31 |
| ATOM | 2348 | O | GLY | A | 296 | 54.778 | 3.798 | 112.609 | 1.00 | 25.86 |
| ATOM | 2349 | N | TYR | A | 297 | 56.005 | 5.034 | 111.185 | 1.00 | 22.83 |
| ATOM | 2350 | CA | TYR | A | 297 | 56.598 | 3.852 | 110.577 | 1.00 | 23.93 |
| ATOM | 2351 | CB | TYR | A | 297 | 56.137 | 3.780 | 109.125 | 1.00 | 21.59 |
| ATOM | 2352 | CG | TYR | A | 297 | 54.660 | 4.084 | 109.035 | 1.00 | 25.85 |
| ATOM | 2353 | CD1 | TYR | A | 297 | 54.203 | 5.402 | 109.017 | 1.00 | 22.28 |
| ATOM | 2354 | CE1 | TYR | A | 297 | 52.842 | 5.695 | 109.089 | 1.00 | 20.19 |
| ATOM | 2355 | CD2 | TYR | A | 297 | 53.713 | 3.062 | 109.116 | 1.00 | 25.28 |
| ATOM | 2356 | CE2 | TYR | A | 297 | 52.352 | 3.346 | 109.190 | 1.00 | 21.83 |
| ATOM | 2357 | CZ | TYR | A | 297 | 51.927 | 4.666 | 109.181 | 1.00 | 21.81 |
| ATOM | 2358 | OH | TYR | A | 297 | 50.588 | 4.972 | 109.305 | 1.00 | 19.51 |
| ATOM | 2359 | C | TYR | A | 297 | 58.104 | 3.694 | 110.674 | 1.00 | 23.78 |
| ATOM | 2360 | O | TYR | A | 297 | 58.665 | 2.724 | 110.154 | 1.00 | 22.07 |
| ATOM | 2361 | N | HIS | A | 298 | 58.765 | 4.641 | 111.326 | 1.00 | 23.71 |
| ATOM | 2362 | CA | HIS | A | 298 | 60.204 | 4.534 | 111.517 | 1.00 | 26.33 |
| ATOM | 2363 | CB | HIS | A | 298 | 60.913 | 5.852 | 111.216 | 1.00 | 28.74 |
| ATOM | 2364 | CG | HIS | A | 298 | 62.403 | 5.727 | 111.213 | 1.00 | 33.08 |
| ATOM | 2365 | CD2 | HIS | A | 298 | 63.273 | 5.465 | 112.215 | 1.00 | 31.83 |
| ATOM | 2366 | ND1 | HIS | A | 298 | 63.151 | 5.775 | 110.056 | 1.00 | 32.49 |
| ATOM | 2367 | CE1 | HIS | A | 298 | 64.419 | 5.547 | 110.345 | 1.00 | 29.10 |
| ATOM | 2368 | NE2 | HIS | A | 298 | 64.520 | 5.354 | 111.648 | 1.00 | 38.70 |
| ATOM | 2369 | C | HIS | A | 298 | 60.371 | 4.188 | 112.996 | 1.00 | 27.81 |
| ATOM | 2370 | O | HIS | A | 298 | 60.120 | 5.020 | 113.865 | 1.00 | 25.07 |
| ATOM | 2371 | N | PRO | A | 299 | 60.829 | 2.963 | 113.297 | 1.00 | 29.37 |
| ATOM | 2372 | CD | PRO | A | 299 | 61.285 | 1.932 | 112.352 | 1.00 | 26.09 |
| ATOM | 2373 | CA | PRO | A | 299 | 61.024 | 2.491 | 114.669 | 1.00 | 29.46 |
| ATOM | 2374 | CB | PRO | A | 299 | 61.675 | 1.118 | 114.465 | 1.00 | 29.03 |
| ATOM | 2375 | CG | PRO | A | 299 | 62.411 | 1.306 | 113.137 | 1.00 | 27.34 |
| ATOM | 2376 | C | PRO | A | 299 | 61.849 | 3.403 | 115.570 | 1.00 | 31.88 |

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Figure 18-37

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 2377 | O | PRO A 299 | 61.480 | 3.622 | 116.724 | 1.00 | 32.45 |
| ATOM | 2378 | N | TYR A 300 | 62.959 | 3.932 | 115.058 | 1.00 | 27.41 |
| ATOM | 2379 | CA | TYR A 300 | 63.803 | 4.801 | 115.878 | 1.00 | 27.34 |
| ATOM | 2380 | CB | TYR A 300 | 65.163 | 5.058 | 115.207 | 1.00 | 26.84 |
| ATOM | 2381 | CG | TYR A 300 | 65.912 | 3.821 | 114.738 | 1.00 | 29.09 |
| ATOM | 2382 | CD1 | TYR A 300 | 65.517 | 2.539 | 115.120 | 1.00 | 30.93 |
| ATOM | 2383 | CE1 | TYR A 300 | 66.214 | 1.411 | 114.682 | 1.00 | 30.68 |
| ATOM | 2384 | CD2 | TYR A 300 | 67.027 | 3.941 | 113.908 | 1.00 | 29.72 |
| ATOM | 2385 | CE2 | TYR A 300 | 67.730 | 2.829 | 113.466 | 1.00 | 30.76 |
| ATOM | 2386 | CZ | TYR A 300 | 67.320 | 1.568 | 113.854 | 1.00 | 33.89 |
| ATOM | 2387 | OH | TYR A 300 | 68.011 | 0.471 | 113.404 | 1.00 | 34.70 |
| ATOM | 2388 | C | TYR A 300 | 63.113 | 6.134 | 116.137 | 1.00 | 23.44 |
| ATOM | 2389 | O | TYR A 300 | 63.108 | 6.631 | 117.264 | 1.00 | 23.87 |
| ATOM | 2390 | N | ALA A 301 | 62.530 | 6.711 | 115.092 | 1.00 | 22.19 |
| ATOM | 2391 | CA | ALA A 301 | 61.839 | 7.993 | 115.216 | 1.00 | 26.50 |
| ATOM | 2392 | CB | ALA A 301 | 61.266 | 8.416 | 113.864 | 1.00 | 24.16 |
| ATOM | 2393 | C | ALA A 301 | 60.715 | 7.878 | 116.237 | 1.00 | 27.86 |
| ATOM | 2394 | O | ALA A 301 | 60.556 | 8.728 | 117.117 | 1.00 | 22.47 |
| ATOM | 2395 | N | LEU A 302 | 59.940 | 6.808 | 116.110 | 1.00 | 23.27 |
| ATOM | 2396 | CA | LEU A 302 | 58.818 | 6.566 | 116.996 | 1.00 | 26.50 |
| ATOM | 2397 | CB | LEU A 302 | 58.036 | 5.354 | 116.483 | 1.00 | 26.02 |
| ATOM | 2398 | CG | LEU A 302 | 56.866 | 4.798 | 117.291 | 1.00 | 29.73 |
| ATOM | 2399 | CD1 | LEU A 302 | 55.983 | 3.938 | 116.394 | 1.00 | 31.31 |
| ATOM | 2400 | CD2 | LEU A 302 | 57.394 | 4.001 | 118.465 | 1.00 | 32.99 |
| ATOM | 2401 | C | LEU A 302 | 59.246 | 6.373 | 118.451 | 1.00 | 27.49 |
| ATOM | 2402 | O | LEU A 302 | 58.648 | 6.946 | 119.358 | 1.00 | 25.22 |
| ATOM | 2403 | N | ALA A 303 | 60.289 | 5.580 | 118.672 | 1.00 | 27.85 |
| ATOM | 2404 | CA | ALA A 303 | 60.765 | 5.320 | 120.024 | 1.00 | 27.33 |
| ATOM | 2405 | CB | ALA A 303 | 61.854 | 4.269 | 119.990 | 1.00 | 29.17 |
| ATOM | 2406 | C | ALA A 303 | 61.279 | 6.580 | 120.714 | 1.00 | 26.64 |
| ATOM | 2407 | O | ALA A 303 | 60.944 | 6.849 | 121.875 | 1.00 | 23.18 |
| ATOM | 2408 | N | ARG A 304 | 62.092 | 7.354 | 120.003 | 1.00 | 27.48 |
| ATOM | 2409 | CA | ARG A 304 | 62.648 | 8.570 | 120.581 | 1.00 | 25.46 |
| ATOM | 2410 | CB | ARG A 304 | 63.773 | 9.136 | 119.704 | 1.00 | 21.31 |
| ATOM | 2411 | CG | ARG A 304 | 65.005 | 8.231 | 119.562 | 1.00 | 25.98 |
| ATOM | 2412 | CD | ARG A 304 | 66.153 | 9.042 | 118.951 | 1.00 | 27.87 |
| ATOM | 2413 | NE | ARG A 304 | 65.647 | 9.766 | 117.796 | 1.00 | 36.76 |
| ATOM | 2414 | CZ | ARG A 304 | 66.207 | 10.838 | 117.261 | 1.00 | 30.79 |
| ATOM | 2415 | NH1 | ARG A 304 | 67.323 | 11.345 | 117.768 | 1.00 | 30.11 |
| ATOM | 2416 | NH2 | ARG A 304 | 65.623 | 11.419 | 116.225 | 1.00 | 36.07 |
| ATOM | 2417 | C | ARG A 304 | 61.585 | 9.634 | 120.803 | 1.00 | 25.46 |
| ATOM | 2418 | O | ARG A 304 | 61.519 | 10.237 | 121.876 | 1.00 | 24.23 |
| ATOM | 2419 | N | ALA A 305 | 60.741 | 9.854 | 119.802 | 1.00 | 22.22 |
| ATOM | 2420 | CA | ALA A 305 | 59.700 | 10.868 | 119.910 | 1.00 | 26.70 |
| ATOM | 2421 | CB | ALA A 305 | 58.914 | 10.960 | 118.607 | 1.00 | 28.14 |
| ATOM | 2422 | C | ALA A 305 | 58.749 | 10.626 | 121.072 | 1.00 | 25.54 |
| ATOM | 2423 | O | ALA A 305 | 58.513 | 11.520 | 121.883 | 1.00 | 24.17 |
| ATOM | 2424 | N | TRP A 306 | 58.189 | 9.426 | 121.160 | 1.00 | 25.66 |
| ATOM | 2425 | CA | TRP A 306 | 57.270 | 9.157 | 122.253 | 1.00 | 28.01 |
| ATOM | 2426 | CB | TRP A 306 | 56.454 | 7.873 | 122.012 | 1.00 | 18.66 |
| ATOM | 2427 | CG | TRP A 306 | 55.382 | 8.052 | 120.973 | 1.00 | 21.80 |
| ATOM | 2428 | CD2 | TRP A 306 | 54.709 | 7.019 | 120.240 | 1.00 | 24.88 |
| ATOM | 2429 | CE2 | TRP A 306 | 53.725 | 7.646 | 119.442 | 1.00 | 23.98 |
| ATOM | 2430 | CE3 | TRP A 306 | 54.839 | 5.623 | 120.181 | 1.00 | 23.26 |
| ATOM | 2431 | CD1 | TRP A 306 | 54.795 | 9.228 | 120.599 | 1.00 | 20.24 |
| ATOM | 2432 | NE1 | TRP A 306 | 53.799 | 8.995 | 119.681 | 1.00 | 24.18 |
| ATOM | 2433 | CZ2 | TRP A 306 | 52.875 | 6.926 | 118.590 | 1.00 | 24.30 |
| ATOM | 2434 | CZ3 | TRP A 306 | 53.993 | 4.906 | 119.335 | 1.00 | 23.89 |
| ATOM | 2435 | CH2 | TRP A 306 | 53.024 | 5.562 | 118.550 | 1.00 | 24.12 |
| ATOM | 2436 | C | TRP A 306 | 57.969 | 9.113 | 123.605 | 1.00 | 27.93 |
| ATOM | 2437 | O | TRP A 306 | 57.330 | 9.319 | 124.637 | 1.00 | 28.58 |
| ATOM | 2438 | N | THR A 307 | 59.273 | 8.851 | 123.615 | 1.00 | 26.76 |
| ATOM | 2439 | CA | THR A 307 | 60.000 | 8.850 | 124.881 | 1.00 | 22.81 |
| ATOM | 2440 | CB | THR A 307 | 61.457 | 8.319 | 124.730 | 1.00 | 25.54 |
| ATOM | 2441 | OG1 | THR A 307 | 61.435 | 6.902 | 124.504 | 1.00 | 22.73 |
| ATOM | 2442 | CG2 | THR A 307 | 62.269 | 8.599 | 125.988 | 1.00 | 24.03 |

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Figure 18-38

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 2443 | C | THR A 307 | 60.027 | 10.288 | 125.396 | 1.00 | 26.54 |
| ATOM | 2444 | O | THR A 307 | 59.925 | 10.526 | 126.604 | 1.00 | 25.34 |
| ATOM | 2445 | N | LEU A 308 | 60.152 | 11.247 | 124.478 | 1.00 | 21.65 |
| ATOM | 2446 | CA | LEU A 308 | 60.172 | 12.657 | 124.862 | 1.00 | 21.41 |
| ATOM | 2447 | CB | LEU A 308 | 60.442 | 13.558 | 123.642 | 1.00 | 19.20 |
| ATOM | 2448 | CG | LEU A 308 | 61.797 | 13.386 | 122.938 | 1.00 | 21.31 |
| ATOM | 2449 | CD1 | LEU A 308 | 61.900 | 14.362 | 121.774 | 1.00 | 21.75 |
| ATOM | 2450 | CD2 | LEU A 308 | 62.937 | 13.622 | 123.915 | 1.00 | 19.26 |
| ATOM | 2451 | C | LEU A 308 | 58.811 | 12.981 | 125.479 | 1.00 | 25.18 |
| ATOM | 2452 | O | LEU A 308 | 58.731 | 13.565 | 126.561 | 1.00 | 21.35 |
| ATOM | 2453 | N | ILE A 309 | 57.743 | 12.567 | 124.806 | 1.00 | 21.74 |
| ATOM | 2454 | CA | ILE A 309 | 56.394 | 12.799 | 125.298 | 1.00 | 19.23 |
| ATOM | 2455 | CB | ILE A 309 | 55.337 | 12.149 | 124.366 | 1.00 | 19.63 |
| ATOM | 2456 | CG2 | ILE A 309 | 53.945 | 12.321 | 124.948 | 1.00 | 19.54 |
| ATOM | 2457 | CG1 | ILE A 309 | 55.403 | 12.788 | 122.979 | 1.00 | 20.80 |
| ATOM | 2458 | CD1 | ILE A 309 | 55.118 | 14.274 | 122.988 | 1.00 | 20.08 |
| ATOM | 2459 | C | ILE A 309 | 56.228 | 12.222 | 126.701 | 1.00 | 23.97 |
| ATOM | 2460 | O | ILE A 309 | 55.731 | 12.894 | 127.602 | 1.00 | 21.38 |
| ATOM | 2461 | N | TRP A 310 | 56.652 | 10.977 | 126.888 | 1.00 | 26.45 |
| ATOM | 2462 | CA | TRP A 310 | 56.525 | 10.342 | 128.192 | 1.00 | 28.35 |
| ATOM | 2463 | CB | TRP A 310 | 56.940 | 8.872 | 128.132 | 1.00 | 23.95 |
| ATOM | 2464 | CG | TRP A 310 | 56.874 | 8.203 | 129.479 | 1.00 | 29.60 |
| ATOM | 2465 | CD2 | TRP A 310 | 55.697 | 7.967 | 130.263 | 1.00 | 31.40 |
| ATOM | 2466 | CE2 | TRP A 310 | 56.115 | 7.390 | 131.480 | 1.00 | 32.47 |
| ATOM | 2467 | CE3 | TRP A 310 | 54.329 | 8.189 | 130.055 | 1.00 | 32.30 |
| ATOM | 2468 | CD1 | TRP A 310 | 57.926 | 7.770 | 130.232 | 1.00 | 33.42 |
| ATOM | 2469 | NE1 | TRP A 310 | 57.480 | 7.282 | 131.436 | 1.00 | 30.09 |
| ATOM | 2470 | CZ2 | TRP A 310 | 55.213 | 7.030 | 132.492 | 1.00 | 29.93 |
| ATOM | 2471 | CZ3 | TRP A 310 | 53.432 | 7.831 | 131.062 | 1.00 | 29.72 |
| ATOM | 2472 | CH2 | TRP A 310 | 53.881 | 7.259 | 132.265 | 1.00 | 24.53 |
| ATOM | 2473 | C | TRP A 310 | 57.308 | 11.048 | 129.293 | 1.00 | 33.49 |
| ATOM | 2474 | O | TRP A 310 | 56.820 | 11.137 | 130.426 | 1.00 | 27.59 |
| ATOM | 2475 | N | CYS A 311 | 58.512 | 11.535 | 128.984 | 1.00 | 29.34 |
| ATOM | 2476 | CA | CYS A 311 | 59.305 | 12.247 | 129.994 | 1.00 | 30.06 |
| ATOM | 2477 | CB | CYS A 311 | 60.722 | 12.538 | 129.479 | 1.00 | 30.08 |
| ATOM | 2478 | SG | CYS A 311 | 61.804 | 11.084 | 129.327 | 1.00 | 33.17 |
| ATOM | 2479 | C | CYS A 311 | 58.612 | 13.560 | 130.397 | 1.00 | 29.25 |
| ATOM | 2480 | O | CYS A 311 | 58.612 | 13.940 | 131.570 | 1.00 | 28.80 |
| ATOM | 2481 | N | GLU A 312 | 58.021 | 14.247 | 129.425 | 1.00 | 23.13 |
| ATOM | 2482 | CA | GLU A 312 | 57.308 | 15.496 | 129.696 | 1.00 | 30.31 |
| ATOM | 2483 | CB | GLU A 312 | 56.648 | 16.032 | 128.427 | 1.00 | 28.97 |
| ATOM | 2484 | CG | GLU A 312 | 57.080 | 17.418 | 127.988 | 1.00 | 41.67 |
| ATOM | 2485 | CD | GLU A 312 | 56.905 | 18.465 | 129.059 | 1.00 | 44.21 |
| ATOM | 2486 | OE1 | GLU A 312 | 55.813 | 18.534 | 129.658 | 1.00 | 54.15 |
| ATOM | 2487 | OE2 | GLU A 312 | 57.860 | 19.233 | 129.290 | 1.00 | 43.90 |
| ATOM | 2488 | C | GLU A 312 | 56.204 | 15.225 | 130.712 | 1.00 | 28.03 |
| ATOM | 2489 | O | GLU A 312 | 56.120 | 15.869 | 131.751 | 1.00 | 30.64 |
| ATOM | 2490 | N | LEU A 313 | 55.343 | 14.270 | 130.388 | 1.00 | 31.06 |
| ATOM | 2491 | CA | LEU A 313 | 54.231 | 13.918 | 131.266 | 1.00 | 36.21 |
| ATOM | 2492 | CB | LEU A 313 | 53.337 | 12.873 | 130.604 | 1.00 | 28.83 |
| ATOM | 2493 | CG | LEU A 313 | 52.493 | 13.342 | 129.429 | 1.00 | 34.62 |
| ATOM | 2494 | CD1 | LEU A 313 | 51.818 | 12.146 | 128.788 | 1.00 | 33.05 |
| ATOM | 2495 | CD2 | LEU A 313 | 51.471 | 14.357 | 129.914 | 1.00 | 27.27 |
| ATOM | 2496 | C | LEU A 313 | 54.685 | 13.377 | 132.610 | 1.00 | 33.97 |
| ATOM | 2497 | O | LEU A 313 | 54.131 | 13.730 | 133.644 | 1.00 | 37.26 |
| ATOM | 2498 | N | SER A 314 | 55.688 | 12.508 | 132.577 | 1.00 | 33.72 |
| ATOM | 2499 | CA | SER A 314 | 56.233 | 11.880 | 133.776 | 1.00 | 33.58 |
| ATOM | 2500 | CB | SER A 314 | 57.183 | 10.743 | 133.388 | 1.00 | 35.88 |
| ATOM | 2501 | OG | SER A 314 | 56.517 | 9.761 | 132.628 | 1.00 | 45.88 |
| ATOM | 2502 | C | SER A 314 | 57.002 | 12.846 | 134.659 | 1.00 | 31.54 |
| ATOM | 2503 | O | SER A 314 | 57.339 | 12.513 | 135.788 | 1.00 | 27.69 |
| ATOM | 2504 | N | GLY A 315 | 57.312 | 14.021 | 134.130 | 1.00 | 35.50 |
| ATOM | 2505 | CA | GLY A 315 | 58.057 | 14.996 | 134.905 | 1.00 | 36.31 |
| ATOM | 2506 | C | GLY A 315 | 59.518 | 14.634 | 135.099 | 1.00 | 38.47 |
| ATOM | 2507 | O | GLY A 315 | 60.138 | 15.049 | 136.078 | 1.00 | 41.57 |
| ATOM | 2508 | N | ARG A 316 | 60.089 | 13.862 | 134.181 | 1.00 | 39.32 |

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Figure 18-39

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 2509 | CA | ARG A 316 | 61.490 | 13.501 | 134.332 | 1.00 | 39.06 |
| ATOM | 2510 | CB | ARG A 316 | 61.641 | 11.982 | 134.413 | 1.00 | 39.16 |
| ATOM | 2511 | CG | ARG A 316 | 61.233 | 11.226 | 133.184 | 1.00 | 39.11 |
| ATOM | 2512 | CD | ARG A 316 | 61.426 | 9.744 | 133.429 | 1.00 | 41.21 |
| ATOM | 2513 | NE | ARG A 316 | 60.461 | 9.229 | 134.389 | 1.00 | 40.97 |
| ATOM | 2514 | CZ | ARG A 316 | 60.524 | 8.021 | 134.926 | 1.00 | 36.40 |
| ATOM | 2515 | NH1 | ARG A 316 | 61.511 | 7.209 | 134.598 | 1.00 | 38.93 |
| ATOM | 2516 | NH2 | ARG A 316 | 59.583 | 7.621 | 135.768 | 1.00 | 30.53 |
| ATOM | 2517 | C | ARG A 316 | 62.369 | 14.083 | 133.230 | 1.00 | 40.17 |
| ATOM | 2518 | O | ARG A 316 | 61.910 | 14.325 | 132.111 | 1.00 | 34.27 |
| ATOM | 2519 | N | GLU A 317 | 63.633 | 14.325 | 133.564 | 1.00 | 41.26 |
| ATOM | 2520 | CA | GLU A 317 | 64.580 | 14.905 | 132.619 | 1.00 | 44.42 |
| ATOM | 2521 | CB | GLU A 317 | 65.901 | 15.249 | 133.317 | 1.00 | 46.84 |
| ATOM | 2522 | CG | GLU A 317 | 65.756 | 15.996 | 134.629 | 1.00 | 57.66 |
| ATOM | 2523 | CD | GLU A 317 | 65.212 | 15.113 | 135.743 | 1.00 | 65.46 |
| ATOM | 2524 | OE1 | GLU A 317 | 65.871 | 14.101 | 136.073 | 1.00 | 68.38 |
| ATOM | 2525 | OE2 | GLU A 317 | 64.129 | 15.425 | 136.287 | 1.00 | 67.24 |
| ATOM | 2526 | C | GLU A 317 | 64.873 | 13.962 | 131.462 | 1.00 | 38.45 |
| ATOM | 2527 | O | GLU A 317 | 64.977 | 12.748 | 131.636 | 1.00 | 38.84 |
| ATOM | 2528 | N | VAL A 318 | 65.010 | 14.525 | 130.275 | 1.00 | 37.64 |
| ATOM | 2529 | CA | VAL A 318 | 65.315 | 13.720 | 129.108 | 1.00 | 39.13 |
| ATOM | 2530 | CB | VAL A 318 | 64.858 | 14.417 | 127.810 | 1.00 | 42.75 |
| ATOM | 2531 | CG1 | VAL A 318 | 65.192 | 13.544 | 126.610 | 1.00 | 41.84 |
| ATOM | 2532 | CG2 | VAL A 318 | 63.364 | 14.701 | 127.867 | 1.00 | 42.38 |
| ATOM | 2533 | C | VAL A 318 | 66.822 | 13.495 | 129.037 | 1.00 | 38.45 |
| ATOM | 2534 | O | VAL A 318 | 67.598 | 14.442 | 128.910 | 1.00 | 36.04 |
| ATOM | 2535 | N | PRO A 319 | 67.261 | 12.236 | 129.156 | 1.00 | 39.54 |
| ATOM | 2536 | CD | PRO A 319 | 66.512 | 10.994 | 129.397 | 1.00 | 40.47 |
| ATOM | 2537 | CA | PRO A 319 | 68.695 | 11.949 | 129.088 | 1.00 | 43.85 |
| ATOM | 2538 | CB | PRO A 319 | 68.745 | 10.439 | 129.319 | 1.00 | 44.12 |
| ATOM | 2539 | CG | PRO A 319 | 67.419 | 9.986 | 128.745 | 1.00 | 46.48 |
| ATOM | 2540 | C | PRO A 319 | 69.228 | 12.353 | 127.718 | 1.00 | 43.55 |
| ATOM | 2541 | O | PRO A 319 | 68.563 | 12.141 | 126.708 | 1.00 | 43.45 |
| ATOM | 2542 | N | GLU A 320 | 70.420 | 12.936 | 127.689 | 1.00 | 42.52 |
| ATOM | 2543 | CA | GLU A 320 | 71.026 | 13.380 | 126.440 | 1.00 | 45.19 |
| ATOM | 2544 | CB | GLU A 320 | 72.384 | 14.032 | 126.706 | 1.00 | 43.86 |
| ATOM | 2545 | CG | GLU A 320 | 73.121 | 14.412 | 125.434 | 1.00 | 52.62 |
| ATOM | 2546 | CD | GLU A 320 | 74.507 | 14.967 | 125.697 | 1.00 | 52.36 |
| ATOM | 2547 | OE1 | GLU A 320 | 75.219 | 15.271 | 124.720 | 1.00 | 56.25 |
| ATOM | 2548 | OE2 | GLU A 320 | 74.883 | 15.101 | 126.875 | 1.00 | 52.25 |
| ATOM | 2549 | C | GLU A 320 | 71.223 | 12.266 | 125.421 | 1.00 | 43.52 |
| ATOM | 2550 | O | GLU A 320 | 70.876 | 12.412 | 124.253 | 1.00 | 41.89 |
| ATOM | 2551 | N | LYS A 321 | 71.781 | 11.150 | 125.867 | 1.00 | 43.35 |
| ATOM | 2552 | CA | LYS A 321 | 72.059 | 10.041 | 124.969 | 1.00 | 43.53 |
| ATOM | 2553 | CB | LYS A 321 | 73.561 | 9.808 | 124.879 | 1.00 | 42.78 |
| ATOM | 2554 | CG | LYS A 321 | 74.238 | 9.340 | 126.180 | 1.00 | 49.38 |
| ATOM | 2555 | CD | LYS A 321 | 74.272 | 10.390 | 127.307 | 1.00 | 57.82 |
| ATOM | 2556 | CE | LYS A 321 | 72.978 | 10.497 | 128.129 | 1.00 | 53.81 |
| ATOM | 2557 | NZ | LYS A 321 | 72.660 | 9.245 | 128.883 | 1.00 | 54.17 |
| ATOM | 2558 | C | LYS A 321 | 71.407 | 8.731 | 125.345 | 1.00 | 41.52 |
| ATOM | 2559 | O | LYS A 321 | 70.954 | 8.540 | 126.469 | 1.00 | 41.98 |
| ATOM | 2560 | N | LEU A 322 | 71.378 | 7.820 | 124.382 | 1.00 | 38.64 |
| ATOM | 2561 | CA | LEU A 322 | 70.815 | 6.508 | 124.613 | 1.00 | 40.46 |
| ATOM | 2562 | CB | LEU A 322 | 70.442 | 5.845 | 123.289 | 1.00 | 42.22 |
| ATOM | 2563 | CG | LEU A 322 | 69.595 | 6.632 | 122.287 | 1.00 | 42.92 |
| ATOM | 2564 | CD1 | LEU A 322 | 69.204 | 5.737 | 121.125 | 1.00 | 41.13 |
| ATOM | 2565 | CD2 | LEU A 322 | 68.361 | 7.148 | 122.967 | 1.00 | 44.41 |
| ATOM | 2566 | C | LEU A 322 | 71.918 | 5.702 | 125.268 | 1.00 | 41.36 |
| ATOM | 2567 | O | LEU A 322 | 73.079 | 5.825 | 124.884 | 1.00 | 44.16 |
| ATOM | 2568 | N | ASN A 323 | 71.579 | 4.894 | 126.265 | 1.00 | 39.89 |
| ATOM | 2569 | CA | ASN A 323 | 72.594 | 4.067 | 126.895 | 1.00 | 40.96 |
| ATOM | 2570 | CB | ASN A 323 | 72.136 | 3.556 | 128.259 | 1.00 | 43.00 |
| ATOM | 2571 | CG | ASN A 323 | 70.787 | 2.886 | 128.202 | 1.00 | 45.59 |
| ATOM | 2572 | OD1 | ASN A 323 | 70.482 | 2.151 | 127.264 | 1.00 | 45.71 |
| ATOM | 2573 | ND2 | ASN A 323 | 69.975 | 3.114 | 129.224 | 1.00 | 48.08 |
| ATOM | 2574 | C | ASN A 323 | 72.828 | 2.894 | 125.954 | 1.00 | 44.88 |

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Figure 18-40

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 2575 | O | ASN A 323 | 72.124 | 2.739 | 124.955 | 1.00 | 46.41 |
| ATOM | 2576 | N | ASN A 324 | 73.809 | 2.062 | 126.268 | 1.00 | 45.98 |
| ATOM | 2577 | CA | ASN A 324 | 74.122 | 0.938 | 125.404 | 1.00 | 49.82 |
| ATOM | 2578 | CB | ASN A 324 | 75.386 | 0.244 | 125.904 | 1.00 | 53.88 |
| ATOM | 2579 | CG | ASN A 324 | 75.960 | -0.711 | 124.888 | 1.00 | 60.09 |
| ATOM | 2580 | OD1 | ASN A 324 | 75.344 | -1.723 | 124.550 | 1.00 | 66.99 |
| ATOM | 2581 | ND2 | ASN A 324 | 77.143 | -0.386 | 124.378 | 1.00 | 58.06 |
| ATOM | 2582 | C | ASN A 324 | 72.979 | -0.070 | 125.267 | 1.00 | 47.12 |
| ATOM | 2583 | O | ASN A 324 | 72.784 | -0.644 | 124.197 | 1.00 | 43.63 |
| ATOM | 2584 | N | LYS A 325 | 72.220 | -0.276 | 126.339 | 1.00 | 46.39 |
| ATOM | 2585 | CA | LYS A 325 | 71.106 | -1.221 | 126.318 | 1.00 | 46.76 |
| ATOM | 2586 | CB | LYS A 325 | 70.428 | -1.328 | 127.695 | 1.00 | 47.65 |
| ATOM | 2587 | CG | LYS A 325 | 71.292 | -1.837 | 128.858 | 1.00 | 54.21 |
| ATOM | 2588 | CD | LYS A 325 | 72.160 | -0.750 | 129.526 | 1.00 | 56.87 |
| ATOM | 2589 | CE | LYS A 325 | 73.329 | -0.289 | 128.671 | 1.00 | 57.45 |
| ATOM | 2590 | NZ | LYS A 325 | 74.091 | 0.816 | 129.307 | 1.00 | 58.32 |
| ATOM | 2591 | C | LYS A 325 | 70.062 | -0.791 | 125.296 | 1.00 | 45.17 |
| ATOM | 2592 | O | LYS A 325 | 69.474 | -1.625 | 124.601 | 1.00 | 42.73 |
| ATOM | 2593 | N | ALA A 326 | 69.832 | 0.514 | 125.213 | 1.00 | 41.43 |
| ATOM | 2594 | CA | ALA A 326 | 68.861 | 1.054 | 124.276 | 1.00 | 41.61 |
| ATOM | 2595 | CB | ALA A 326 | 68.562 | 2.508 | 124.616 | 1.00 | 42.80 |
| ATOM | 2596 | C | ALA A 326 | 69.365 | 0.940 | 122.838 | 1.00 | 43.80 |
| ATOM | 2597 | O | ALA A 326 | 68.595 | 0.625 | 121.926 | 1.00 | 45.17 |
| ATOM | 2598 | N | LYS A 327 | 70.658 | 1.191 | 122.637 | 1.00 | 43.46 |
| ATOM | 2599 | CA | LYS A 327 | 71.235 | 1.120 | 121.296 | 1.00 | 43.26 |
| ATOM | 2600 | CB | LYS A 327 | 72.723 | 1.484 | 121.311 | 1.00 | 44.77 |
| ATOM | 2601 | CG | LYS A 327 | 73.037 | 2.892 | 121.800 | 1.00 | 50.87 |
| ATOM | 2602 | CD | LYS A 327 | 74.544 | 3.168 | 121.747 | 1.00 | 52.74 |
| ATOM | 2603 | CE | LYS A 327 | 74.916 | 4.508 | 122.377 | 1.00 | 51.30 |
| ATOM | 2604 | NZ | LYS A 327 | 74.256 | 5.670 | 121.715 | 1.00 | 52.72 |
| ATOM | 2605 | C | LYS A 327 | 71.063 | -0.274 | 120.728 | 1.00 | 41.29 |
| ATOM | 2606 | O | LYS A 327 | 70.625 | -0.437 | 119.592 | 1.00 | 38.83 |
| ATOM | 2607 | N | GLU A 328 | 71.403 | -1.278 | 121.526 | 1.00 | 39.95 |
| ATOM | 2608 | CA | GLU A 328 | 71.276 | -2.660 | 121.090 | 1.00 | 42.40 |
| ATOM | 2609 | CB | GLU A 328 | 71.875 | -3.605 | 122.135 | 1.00 | 43.05 |
| ATOM | 2610 | CG | GLU A 328 | 73.369 | -3.432 | 122.295 | 1.00 | 48.81 |
| ATOM | 2611 | CD | GLU A 328 | 74.096 | -3.529 | 120.963 | 1.00 | 52.11 |
| ATOM | 2612 | OE1 | GLU A 328 | 73.972 | -4.574 | 120.291 | 1.00 | 55.44 |
| ATOM | 2613 | OE2 | GLU A 328 | 74.785 | -2.558 | 120.584 | 1.00 | 51.64 |
| ATOM | 2614 | C | GLU A 328 | 69.825 | -3.030 | 120.818 | 1.00 | 39.51 |
| ATOM | 2615 | O | GLU A 328 | 69.536 | -3.842 | 119.939 | 1.00 | 37.35 |
| ATOM | 2616 | N | LEU A 329 | 68.911 | -2.444 | 121.582 | 1.00 | 36.37 |
| ATOM | 2617 | CA | LEU A 329 | 67.496 | -2.717 | 121.380 | 1.00 | 36.03 |
| ATOM | 2618 | CB | LEU A 329 | 66.646 | -1.958 | 122.400 | 1.00 | 34.66 |
| ATOM | 2619 | CG | LEU A 329 | 65.133 | -2.110 | 122.213 | 1.00 | 33.88 |
| ATOM | 2620 | CD1 | LEU A 329 | 64.755 | -3.572 | 122.351 | 1.00 | 36.21 |
| ATOM | 2621 | CD2 | LEU A 329 | 64.391 | -1.268 | 123.240 | 1.00 | 34.00 |
| ATOM | 2622 | C | LEU A 329 | 67.120 | -2.268 | 119.971 | 1.00 | 33.64 |
| ATOM | 2623 | O | LEU A 329 | 66.655 | -3.061 | 119.162 | 1.00 | 31.29 |
| ATOM | 2624 | N | LEU A 330 | 67.333 | -0.990 | 119.681 | 1.00 | 33.78 |
| ATOM | 2625 | CA | LEU A 330 | 67.004 | -0.461 | 118.366 | 1.00 | 36.38 |
| ATOM | 2626 | CB | LEU A 330 | 67.326 | 1.033 | 118.294 | 1.00 | 30.74 |
| ATOM | 2627 | CG | LEU A 330 | 66.514 | 1.958 | 119.205 | 1.00 | 31.51 |
| ATOM | 2628 | CD1 | LEU A 330 | 66.857 | 3.404 | 118.894 | 1.00 | 22.11 |
| ATOM | 2629 | CD2 | LEU A 330 | 65.028 | 1.728 | 118.978 | 1.00 | 29.69 |
| ATOM | 2630 | C | LEU A 330 | 67.729 | -1.201 | 117.246 | 1.00 | 36.49 |
| ATOM | 2631 | O | LEU A 330 | 67.142 | -1.493 | 116.210 | 1.00 | 35.61 |
| ATOM | 2632 | N | LYS A 331 | 69.005 | -1.503 | 117.455 | 1.00 | 37.63 |
| ATOM | 2633 | CA | LYS A 331 | 69.786 | -2.205 | 116.446 | 1.00 | 41.32 |
| ATOM | 2634 | CB | LYS A 331 | 71.256 | -2.272 | 116.874 | 1.00 | 44.74 |
| ATOM | 2635 | CG | LYS A 331 | 71.954 | -0.919 | 116.869 | 1.00 | 44.68 |
| ATOM | 2636 | CD | LYS A 331 | 73.350 | -0.964 | 117.498 | 1.00 | 51.42 |
| ATOM | 2637 | CE | LYS A 331 | 74.315 | -1.889 | 116.765 | 1.00 | 53.71 |
| ATOM | 2638 | NZ | LYS A 331 | 73.928 | -3.327 | 116.855 | 1.00 | 56.15 |
| ATOM | 2639 | C | LYS A 331 | 69.258 | -3.612 | 116.173 | 1.00 | 42.35 |
| ATOM | 2640 | O | LYS A 331 | 69.310 | -4.086 | 115.042 | 1.00 | 42.68 |

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Figure 18-41

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 2641 | N | SER A 332 | 68.734 | -4.270 | 117.200 | 1.00 | 41.56 |
| ATOM | 2642 | CA | SER A 332 | 68.226 | -5.629 | 117.039 | 1.00 | 46.88 |
| ATOM | 2643 | CB | SER A 332 | 68.045 | -6.298 | 118.400 | 1.00 | 42.19 |
| ATOM | 2644 | OG | SER A 332 | 66.959 | -5.714 | 119.096 | 1.00 | 39.55 |
| ATOM | 2645 | C | SER A 332 | 66.896 | -5.687 | 116.297 | 1.00 | 48.58 |
| ATOM | 2646 | O | SER A 332 | 66.393 | -6.774 | 116.017 | 1.00 | 45.78 |
| ATOM | 2647 | N | ILE A 333 | 66.325 | -4.531 | 115.979 | 1.00 | 48.27 |
| ATOM | 2648 | CA | ILE A 333 | 65.041 | -4.503 | 115.292 | 1.00 | 51.82 |
| ATOM | 2649 | CB | ILE A 333 | 64.378 | -3.119 | 115.402 | 1.00 | 52.16 |
| ATOM | 2650 | CG2 | ILE A 333 | 63.038 | -3.122 | 114.683 | 1.00 | 52.64 |
| ATOM | 2651 | CG1 | ILE A 333 | 64.163 | -2.765 | 116.871 | 1.00 | 52.70 |
| ATOM | 2652 | CD1 | ILE A 333 | 63.550 | -1.402 | 117.077 | 1.00 | 56.70 |
| ATOM | 2653 | C | ILE A 333 | 65.112 | -4.887 | 113.820 | 1.00 | 53.43 |
| ATOM | 2654 | O | ILE A 333 | 66.118 | -4.675 | 113.145 | 1.00 | 56.45 |
| ATOM | 2655 | N | ASP A 334 | 64.016 | -5.461 | 113.344 | 1.00 | 55.53 |
| ATOM | 2656 | CA | ASP A 334 | 63.865 | -5.892 | 111.962 | 1.00 | 59.58 |
| ATOM | 2657 | CB | ASP A 334 | 62.845 | -7.040 | 111.918 | 1.00 | 62.69 |
| ATOM | 2658 | CG | ASP A 334 | 61.546 | -6.712 | 112.664 | 1.00 | 66.23 |
| ATOM | 2659 | OD1 | ASP A 334 | 60.795 | -5.814 | 112.227 | 1.00 | 63.25 |
| ATOM | 2660 | OD2 | ASP A 334 | 61.277 | -7.354 | 113.704 | 1.00 | 63.45 |
| ATOM | 2661 | C | ASP A 334 | 63.385 | -4.705 | 111.125 | 1.00 | 60.81 |
| ATOM | 2662 | O | ASP A 334 | 62.239 | -4.673 | 110.681 | 1.00 | 59.47 |
| ATOM | 2663 | N | PHE A 335 | 64.266 | -3.736 | 110.889 | 1.00 | 60.00 |
| ATOM | 2664 | CA | PHE A 335 | 63.864 | -2.545 | 110.147 | 1.00 | 59.37 |
| ATOM | 2665 | CB | PHE A 335 | 64.247 | -1.298 | 110.952 | 1.00 | 53.38 |
| ATOM | 2666 | CG | PHE A 335 | 63.895 | -0.013 | 110.275 | 1.00 | 49.13 |
| ATOM | 2667 | CD1 | PHE A 335 | 62.618 | 0.189 | 109.770 | 1.00 | 44.32 |
| ATOM | 2668 | CD2 | PHE A 335 | 64.845 | 0.993 | 110.127 | 1.00 | 49.91 |
| ATOM | 2669 | CE1 | PHE A 335 | 62.288 | 1.373 | 109.122 | 1.00 | 42.74 |
| ATOM | 2670 | CE2 | PHE A 335 | 64.526 | 2.180 | 109.483 | 1.00 | 46.40 |
| ATOM | 2671 | CZ | PHE A 335 | 63.244 | 2.370 | 108.978 | 1.00 | 42.77 |
| ATOM | 2672 | C | PHE A 335 | 64.334 | -2.399 | 108.696 | 1.00 | 60.85 |
| ATOM | 2673 | O | PHE A 335 | 63.689 | -2.914 | 107.785 | 1.00 | 66.28 |
| ATOM | 2674 | N | GLU A 336 | 65.430 | -1.671 | 108.493 | 1.00 | 57.40 |
| ATOM | 2675 | CA | GLU A 336 | 66.015 | -1.411 | 107.174 | 1.00 | 58.96 |
| ATOM | 2676 | CB | GLU A 336 | 65.782 | -2.579 | 106.211 | 1.00 | 62.66 |
| ATOM | 2677 | CG | GLU A 336 | 66.417 | -2.377 | 104.846 | 1.00 | 68.51 |
| ATOM | 2678 | CD | GLU A 336 | 66.277 | -3.590 | 103.943 | 1.00 | 73.21 |
| ATOM | 2679 | OE1 | GLU A 336 | 66.753 | -4.678 | 104.333 | 1.00 | 73.30 |
| ATOM | 2680 | OE2 | GLU A 336 | 65.697 | -3.457 | 102.843 | 1.00 | 75.74 |
| ATOM | 2681 | C | GLU A 336 | 65.460 | -0.124 | 106.576 | 1.00 | 55.70 |
| ATOM | 2682 | O | GLU A 336 | 64.281 | -0.023 | 106.253 | 1.00 | 55.28 |
| ATOM | 2683 | N | GLU A 337 | 66.338 | 0.857 | 106.432 | 1.00 | 54.75 |
| ATOM | 2684 | CA | GLU A 337 | 65.986 | 2.167 | 105.905 | 1.00 | 55.99 |
| ATOM | 2685 | CB | GLU A 337 | 67.221 | 3.065 | 105.983 | 1.00 | 51.75 |
| ATOM | 2686 | CG | GLU A 337 | 66.926 | 4.536 | 106.092 | 1.00 | 52.28 |
| ATOM | 2687 | CD | GLU A 337 | 66.184 | 4.891 | 107.366 | 1.00 | 43.72 |
| ATOM | 2688 | OE1 | GLU A 337 | 66.705 | 4.640 | 108.474 | 1.00 | 42.21 |
| ATOM | 2689 | OE2 | GLU A 337 | 65.072 | 5.425 | 107.256 | 1.00 | 47.31 |
| ATOM | 2690 | C | GLU A 337 | 65.485 | 2.064 | 104.460 | 1.00 | 57.56 |
| ATOM | 2691 | O | GLU A 337 | 66.087 | 1.377 | 103.639 | 1.00 | 58.29 |
| ATOM | 2692 | N | PHE A 338 | 64.385 | 2.745 | 104.151 | 1.00 | 60.26 |
| ATOM | 2693 | CA | PHE A 338 | 63.814 | 2.710 | 102.805 | 1.00 | 61.69 |
| ATOM | 2694 | CB | PHE A 338 | 62.561 | 3.582 | 102.723 | 1.00 | 60.86 |
| ATOM | 2695 | CG | PHE A 338 | 61.845 | 3.493 | 101.401 | 1.00 | 61.92 |
| ATOM | 2696 | CD1 | PHE A 338 | 61.054 | 2.391 | 101.094 | 1.00 | 62.99 |
| ATOM | 2697 | CD2 | PHE A 338 | 61.970 | 4.508 | 100.458 | 1.00 | 62.74 |
| ATOM | 2698 | CE1 | PHE A 338 | 60.392 | 2.302 | 99.868 | 1.00 | 65.11 |
| ATOM | 2699 | CE2 | PHE A 338 | 61.315 | 4.428 | 99.228 | 1.00 | 64.62 |
| ATOM | 2700 | CZ | PHE A 338 | 60.523 | 3.322 | 98.934 | 1.00 | 63.87 |
| ATOM | 2701 | C | PHE A 338 | 64.818 | 3.208 | 101.773 | 1.00 | 64.33 |
| ATOM | 2702 | O | PHE A 338 | 64.803 | 2.781 | 100.616 | 1.00 | 62.45 |
| ATOM | 2703 | N | ASP A 339 | 65.677 | 4.130 | 102.194 | 1.00 | 64.11 |
| ATOM | 2704 | CA | ASP A 339 | 66.689 | 4.684 | 101.310 | 1.00 | 67.42 |
| ATOM | 2705 | CB | ASP A 339 | 66.565 | 6.206 | 101.248 | 1.00 | 67.20 |
| ATOM | 2706 | CG | ASP A 339 | 67.647 | 6.838 | 100.402 | 1.00 | 68.03 |

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Figure 18-42

| | | | | | | | |
|------|------|---------------|--------|--------|---------|------|-------|
| ATOM | 2707 | OD1 ASP A 339 | 67.796 | 6.432 | 99.229 | 1.00 | 72.20 |
| ATOM | 2708 | OD2 ASP A 339 | 68.346 | 7.740 | 100.904 | 1.00 | 64.15 |
| ATOM | 2709 | C ASP A 339 | 68.088 | 4.295 | 101.763 | 1.00 | 68.73 |
| ATOM | 2710 | O ASP A 339 | 68.511 | 4.628 | 102.869 | 1.00 | 68.17 |
| ATOM | 2711 | N ASP A 340 | 68.796 | 3.588 | 100.888 | 1.00 | 71.90 |
| ATOM | 2712 | CA ASP A 340 | 70.151 | 3.111 | 101.149 | 1.00 | 73.59 |
| ATOM | 2713 | CB ASP A 340 | 70.778 | 2.601 | 99.848 | 1.00 | 75.47 |
| ATOM | 2714 | CG ASP A 340 | 69.953 | 1.511 | 99.195 | 1.00 | 76.03 |
| ATOM | 2715 | OD1 ASP A 340 | 69.761 | 0.449 | 99.823 | 1.00 | 76.90 |
| ATOM | 2716 | OD2 ASP A 340 | 69.492 | 1.718 | 98.054 | 1.00 | 80.23 |
| ATOM | 2717 | C ASP A 340 | 71.069 | 4.155 | 101.766 | 1.00 | 72.77 |
| ATOM | 2718 | O ASP A 340 | 71.618 | 3.946 | 102.845 | 1.00 | 73.08 |
| ATOM | 2719 | N GLU A 341 | 71.242 | 5.275 | 101.074 | 1.00 | 73.15 |
| ATOM | 2720 | CA GLU A 341 | 72.112 | 6.341 | 101.557 | 1.00 | 74.56 |
| ATOM | 2721 | CB GLU A 341 | 72.917 | 6.924 | 100.390 | 1.00 | 77.06 |
| ATOM | 2722 | CG GLU A 341 | 73.878 | 8.034 | 100.792 | 1.00 | 82.57 |
| ATOM | 2723 | CD GLU A 341 | 74.924 | 7.571 | 101.794 | 1.00 | 85.34 |
| ATOM | 2724 | OE1 GLU A 341 | 75.718 | 6.669 | 101.450 | 1.00 | 86.64 |
| ATOM | 2725 | OE2 GLU A 341 | 74.951 | 8.106 | 102.924 | 1.00 | 85.37 |
| ATOM | 2726 | C GLU A 341 | 71.327 | 7.453 | 102.245 | 1.00 | 72.47 |
| ATOM | 2727 | O GLU A 341 | 70.822 | 8.364 | 101.589 | 1.00 | 76.75 |
| ATOM | 2728 | N VAL A 342 | 71.228 | 7.381 | 103.566 | 1.00 | 67.86 |
| ATOM | 2729 | CA VAL A 342 | 70.503 | 8.393 | 104.323 | 1.00 | 64.84 |
| ATOM | 2730 | CB VAL A 342 | 69.160 | 7.853 | 104.850 | 1.00 | 66.27 |
| ATOM | 2731 | CG1 VAL A 342 | 68.256 | 7.494 | 103.701 | 1.00 | 67.95 |
| ATOM | 2732 | CG2 VAL A 342 | 69.400 | 6.637 | 105.722 | 1.00 | 65.37 |
| ATOM | 2733 | C VAL A 342 | 71.305 | 8.871 | 105.520 | 1.00 | 61.75 |
| ATOM | 2734 | O VAL A 342 | 71.375 | 10.066 | 105.795 | 1.00 | 64.14 |
| ATOM | 2735 | N ASP A 343 | 71.912 | 7.925 | 106.225 | 1.00 | 56.79 |
| ATOM | 2736 | CA ASP A 343 | 72.692 | 8.229 | 107.417 | 1.00 | 54.53 |
| ATOM | 2737 | CB ASP A 343 | 73.707 | 9.340 | 107.158 | 1.00 | 56.31 |
| ATOM | 2738 | CG ASP A 343 | 74.531 | 9.660 | 108.388 | 1.00 | 58.81 |
| ATOM | 2739 | OD1 ASP A 343 | 75.298 | 10.644 | 108.357 | 1.00 | 65.36 |
| ATOM | 2740 | OD2 ASP A 343 | 74.420 | 8.918 | 109.387 | 1.00 | 54.29 |
| ATOM | 2741 | C ASP A 343 | 71.765 | 8.675 | 108.534 | 1.00 | 50.70 |
| ATOM | 2742 | O ASP A 343 | 71.442 | 9.859 | 108.651 | 1.00 | 46.00 |
| ATOM | 2743 | N ARG A 344 | 71.328 | 7.717 | 109.341 | 1.00 | 46.20 |
| ATOM | 2744 | CA ARG A 344 | 70.452 | 8.004 | 110.463 | 1.00 | 41.18 |
| ATOM | 2745 | CB ARG A 344 | 69.121 | 7.268 | 110.299 | 1.00 | 39.81 |
| ATOM | 2746 | CG ARG A 344 | 68.289 | 7.711 | 109.098 | 1.00 | 35.08 |
| ATOM | 2747 | CD ARG A 344 | 68.036 | 9.211 | 109.121 | 1.00 | 28.37 |
| ATOM | 2748 | NE ARG A 344 | 67.157 | 9.645 | 108.036 | 1.00 | 30.90 |
| ATOM | 2749 | CZ ARG A 344 | 67.013 | 10.909 | 107.649 | 1.00 | 31.05 |
| ATOM | 2750 | NH1 ARG A 344 | 67.693 | 11.874 | 108.258 | 1.00 | 30.49 |
| ATOM | 2751 | NH2 ARG A 344 | 66.201 | 11.212 | 106.646 | 1.00 | 31.76 |
| ATOM | 2752 | C ARG A 344 | 71.147 | 7.561 | 111.742 | 1.00 | 38.46 |
| ATOM | 2753 | O ARG A 344 | 70.516 | 7.370 | 112.773 | 1.00 | 34.99 |
| ATOM | 2754 | N SER A 345 | 72.464 | 7.418 | 111.662 | 1.00 | 33.97 |
| ATOM | 2755 | CA SER A 345 | 73.261 | 6.981 | 112.795 | 1.00 | 33.68 |
| ATOM | 2756 | CB SER A 345 | 74.742 | 6.972 | 112.404 | 1.00 | 39.11 |
| ATOM | 2757 | OG SER A 345 | 75.163 | 8.260 | 111.990 | 1.00 | 42.80 |
| ATOM | 2758 | C SER A 345 | 73.054 | 7.826 | 114.053 | 1.00 | 31.83 |
| ATOM | 2759 | O SER A 345 | 73.100 | 7.314 | 115.167 | 1.00 | 24.35 |
| ATOM | 2760 | N TYR A 346 | 72.819 | 9.119 | 113.877 | 1.00 | 33.10 |
| ATOM | 2761 | CA TYR A 346 | 72.614 | 10.003 | 115.015 | 1.00 | 34.50 |
| ATOM | 2762 | CB TYR A 346 | 72.397 | 11.437 | 114.522 | 1.00 | 35.16 |
| ATOM | 2763 | CG TYR A 346 | 71.168 | 11.615 | 113.659 | 1.00 | 39.69 |
| ATOM | 2764 | CD1 TYR A 346 | 69.909 | 11.814 | 114.227 | 1.00 | 36.57 |
| ATOM | 2765 | CE1 TYR A 346 | 68.767 | 11.940 | 113.424 | 1.00 | 40.23 |
| ATOM | 2766 | CD2 TYR A 346 | 71.260 | 11.544 | 112.270 | 1.00 | 39.04 |
| ATOM | 2767 | CE2 TYR A 346 | 70.131 | 11.667 | 111.463 | 1.00 | 38.65 |
| ATOM | 2768 | CZ TYR A 346 | 68.890 | 11.864 | 112.041 | 1.00 | 37.64 |
| ATOM | 2769 | OH TYR A 346 | 67.776 | 11.982 | 111.234 | 1.00 | 32.48 |
| ATOM | 2770 | C TYR A 346 | 71.432 | 9.560 | 115.874 | 1.00 | 37.72 |
| ATOM | 2771 | O TYR A 346 | 71.396 | 9.829 | 117.074 | 1.00 | 35.48 |
| ATOM | 2772 | N MET A 347 | 70.472 | 8.869 | 115.265 | 1.00 | 35.36 |

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Figure 18-43

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 2773 | CA | MET | A | 347 | 69.295 | 8.418 | 116.004 | 1.00 | 36.97 |
| ATOM | 2774 | CB | MET | A | 347 | 68.226 | 7.868 | 115.052 | 1.00 | 33.45 |
| ATOM | 2775 | CG | MET | A | 347 | 67.853 | 8.809 | 113.921 | 1.00 | 28.09 |
| ATOM | 2776 | SD | MET | A | 347 | 66.471 | 8.194 | 112.943 | 1.00 | 32.14 |
| ATOM | 2777 | CE | MET | A | 347 | 67.058 | 6.647 | 112.457 | 1.00 | 39.25 |
| ATOM | 2778 | C | MET | A | 347 | 69.632 | 7.363 | 117.055 | 1.00 | 34.67 |
| ATOM | 2779 | O | MET | A | 347 | 68.890 | 7.187 | 118.016 | 1.00 | 33.46 |
| ATOM | 2780 | N | LEU | A | 348 | 70.747 | 6.663 | 116.880 | 1.00 | 36.42 |
| ATOM | 2781 | CA | LEU | A | 348 | 71.137 | 5.641 | 117.846 | 1.00 | 34.57 |
| ATOM | 2782 | CB | LEU | A | 348 | 71.841 | 4.476 | 117.152 | 1.00 | 34.16 |
| ATOM | 2783 | CG | LEU | A | 348 | 71.066 | 3.655 | 116.121 | 1.00 | 35.61 |
| ATOM | 2784 | CD1 | LEU | A | 348 | 72.010 | 2.660 | 115.469 | 1.00 | 36.58 |
| ATOM | 2785 | CD2 | LEU | A | 348 | 69.906 | 2.935 | 116.788 | 1.00 | 42.34 |
| ATOM | 2786 | C | LEU | A | 348 | 72.075 | 6.232 | 118.885 | 1.00 | 37.10 |
| ATOM | 2787 | O | LEU | A | 348 | 72.583 | 5.513 | 119.745 | 1.00 | 37.75 |
| ATOM | 2788 | N | GLU | A | 349 | 72.295 | 7.541 | 118.801 | 1.00 | 38.31 |
| ATOM | 2789 | CA | GLU | A | 349 | 73.192 | 8.231 | 119.726 | 1.00 | 42.86 |
| ATOM | 2790 | CB | GLU | A | 349 | 74.150 | 9.136 | 118.948 | 1.00 | 47.04 |
| ATOM | 2791 | CG | GLU | A | 349 | 74.942 | 8.426 | 117.867 | 1.00 | 53.27 |
| ATOM | 2792 | CD | GLU | A | 349 | 75.828 | 7.325 | 118.410 | 1.00 | 58.36 |
| ATOM | 2793 | OE1 | GLU | A | 349 | 76.681 | 7.619 | 119.279 | 1.00 | 59.59 |
| ATOM | 2794 | OE2 | GLU | A | 349 | 75.669 | 6.166 | 117.963 | 1.00 | 59.17 |
| ATOM | 2795 | C | GLU | A | 349 | 72.458 | 9.080 | 120.752 | 1.00 | 41.72 |
| ATOM | 2796 | O | GLU | A | 349 | 72.564 | 8.852 | 121.959 | 1.00 | 42.27 |
| ATOM | 2797 | N | THR | A | 350 | 71.716 | 10.067 | 120.261 | 1.00 | 37.05 |
| ATOM | 2798 | CA | THR | A | 350 | 70.992 | 10.976 | 121.135 | 1.00 | 40.78 |
| ATOM | 2799 | CB | THR | A | 350 | 71.468 | 12.418 | 120.900 | 1.00 | 41.69 |
| ATOM | 2800 | OG1 | THR | A | 350 | 71.359 | 12.733 | 119.508 | 1.00 | 43.25 |
| ATOM | 2801 | CG2 | THR | A | 350 | 72.918 | 12.575 | 121.325 | 1.00 | 44.11 |
| ATOM | 2802 | C | THR | A | 350 | 69.474 | 10.911 | 120.968 | 1.00 | 41.47 |
| ATOM | 2803 | O | THR | A | 350 | 68.968 | 10.608 | 119.884 | 1.00 | 39.72 |
| ATOM | 2804 | N | LEU | A | 351 | 68.760 | 11.199 | 122.054 | 1.00 | 38.68 |
| ATOM | 2805 | CA | LEU | A | 351 | 67.299 | 11.185 | 122.056 | 1.00 | 35.91 |
| ATOM | 2806 | CB | LEU | A | 351 | 66.763 | 11.210 | 123.487 | 1.00 | 35.94 |
| ATOM | 2807 | CG | LEU | A | 351 | 66.752 | 9.890 | 124.251 | 1.00 | 37.67 |
| ATOM | 2808 | CD1 | LEU | A | 351 | 66.290 | 10.118 | 125.677 | 1.00 | 40.11 |
| ATOM | 2809 | CD2 | LEU | A | 351 | 65.813 | 8.920 | 123.544 | 1.00 | 39.29 |
| ATOM | 2810 | C | LEU | A | 351 | 66.679 | 12.342 | 121.294 | 1.00 | 37.76 |
| ATOM | 2811 | O | LEU | A | 351 | 65.747 | 12.149 | 120.512 | 1.00 | 34.86 |
| ATOM | 2812 | N | LYS | A | 352 | 67.192 | 13.544 | 121.525 | 1.00 | 34.79 |
| ATOM | 2813 | CA | LYS | A | 352 | 66.651 | 14.724 | 120.870 | 1.00 | 38.73 |
| ATOM | 2814 | CB | LYS | A | 352 | 66.676 | 15.911 | 121.835 | 1.00 | 36.48 |
| ATOM | 2815 | CG | LYS | A | 352 | 66.062 | 15.580 | 123.179 | 1.00 | 42.08 |
| ATOM | 2816 | CD | LYS | A | 352 | 66.202 | 16.701 | 124.196 | 1.00 | 43.22 |
| ATOM | 2817 | CE | LYS | A | 352 | 65.349 | 17.901 | 123.845 | 1.00 | 49.81 |
| ATOM | 2818 | NZ | LYS | A | 352 | 65.342 | 18.880 | 124.972 | 1.00 | 52.70 |
| ATOM | 2819 | C | LYS | A | 352 | 67.425 | 15.063 | 119.610 | 1.00 | 38.77 |
| ATOM | 2820 | O | LYS | A | 352 | 68.654 | 15.098 | 119.601 | 1.00 | 36.21 |
| ATOM | 2821 | N | ASP | A | 353 | 66.697 | 15.293 | 118.530 | 1.00 | 37.69 |
| ATOM | 2822 | CA | ASP | A | 353 | 67.337 | 15.647 | 117.286 | 1.00 | 39.89 |
| ATOM | 2823 | CB | ASP | A | 353 | 66.532 | 15.075 | 116.110 | 1.00 | 43.53 |
| ATOM | 2824 | CG | ASP | A | 353 | 65.058 | 15.368 | 116.211 | 1.00 | 47.99 |
| ATOM | 2825 | OD1 | ASP | A | 353 | 64.253 | 14.623 | 115.593 | 1.00 | 38.06 |
| ATOM | 2826 | OD2 | ASP | A | 353 | 64.706 | 16.352 | 116.898 | 1.00 | 52.94 |
| ATOM | 2827 | C | ASP | A | 353 | 67.457 | 17.165 | 117.247 | 1.00 | 39.20 |
| ATOM | 2828 | O | ASP | A | 353 | 66.890 | 17.861 | 118.092 | 1.00 | 35.66 |
| ATOM | 2829 | N | PRO | A | 354 | 68.244 | 17.696 | 116.302 | 1.00 | 40.75 |
| ATOM | 2830 | CD | PRO | A | 354 | 69.047 | 17.005 | 115.279 | 1.00 | 40.05 |
| ATOM | 2831 | CA | PRO | A | 354 | 68.426 | 19.145 | 116.179 | 1.00 | 38.41 |
| ATOM | 2832 | CB | PRO | A | 354 | 69.534 | 19.250 | 115.140 | 1.00 | 36.24 |
| ATOM | 2833 | CG | PRO | A | 354 | 69.190 | 18.095 | 114.225 | 1.00 | 39.41 |
| ATOM | 2834 | C | PRO | A | 354 | 67.144 | 19.780 | 115.689 | 1.00 | 37.28 |
| ATOM | 2835 | O | PRO | A | 354 | 66.299 | 19.106 | 115.094 | 1.00 | 31.87 |
| ATOM | 2836 | N | TRP | A | 355 | 66.993 | 21.074 | 115.934 | 1.00 | 37.87 |
| ATOM | 2837 | CA | TRP | A | 355 | 65.804 | 21.757 | 115.472 | 1.00 | 40.04 |
| ATOM | 2838 | CB | TRP | A | 355 | 65.714 | 23.157 | 116.080 | 1.00 | 42.85 |

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Figure 18-44

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 2839 | CG | TRP | A | 355 | 64.333 | 23.471 | 116.569 | 1.00 | 53.01 |
| ATOM | 2840 | CD2 | TRP | A | 355 | 63.439 | 24.463 | 116.047 | 1.00 | 54.23 |
| ATOM | 2841 | CE2 | TRP | A | 355 | 62.234 | 24.368 | 116.783 | 1.00 | 52.59 |
| ATOM | 2842 | CE3 | TRP | A | 355 | 63.538 | 25.422 | 115.028 | 1.00 | 52.82 |
| ATOM | 2843 | CD1 | TRP | A | 355 | 63.655 | 22.836 | 117.575 | 1.00 | 51.80 |
| ATOM | 2844 | NE1 | TRP | A | 355 | 62.393 | 23.368 | 117.708 | 1.00 | 51.38 |
| ATOM | 2845 | CZ2 | TRP | A | 355 | 61.134 | 25.197 | 116.532 | 1.00 | 51.28 |
| ATOM | 2846 | CZ3 | TRP | A | 355 | 62.444 | 26.245 | 114.779 | 1.00 | 53.22 |
| ATOM | 2847 | CH2 | TRP | A | 355 | 61.257 | 26.126 | 115.531 | 1.00 | 50.50 |
| ATOM | 2848 | C | TRP | A | 355 | 65.935 | 21.836 | 113.954 | 1.00 | 37.34 |
| ATOM | 2849 | O | TRP | A | 355 | 67.041 | 21.929 | 113.422 | 1.00 | 39.01 |
| ATOM | 2850 | N | ARG | A | 356 | 64.809 | 21.764 | 113.259 | 1.00 | 36.31 |
| ATOM | 2851 | CA | ARG | A | 356 | 64.797 | 21.820 | 111.802 | 1.00 | 35.22 |
| ATOM | 2852 | CB | ARG | A | 356 | 64.317 | 20.469 | 111.252 | 1.00 | 33.36 |
| ATOM | 2853 | CG | ARG | A | 356 | 65.310 | 19.340 | 111.564 | 1.00 | 34.50 |
| ATOM | 2854 | CD | ARG | A | 356 | 64.729 | 17.927 | 111.468 | 1.00 | 28.06 |
| ATOM | 2855 | NE | ARG | A | 356 | 65.745 | 16.956 | 111.870 | 1.00 | 24.79 |
| ATOM | 2856 | CZ | ARG | A | 356 | 65.499 | 15.703 | 112.236 | 1.00 | 27.56 |
| ATOM | 2857 | NH1 | ARG | A | 356 | 64.253 | 15.237 | 112.259 | 1.00 | 19.09 |
| ATOM | 2858 | NH2 | ARG | A | 356 | 66.502 | 14.918 | 112.604 | 1.00 | 21.34 |
| ATOM | 2859 | C | ARG | A | 356 | 63.874 | 22.955 | 111.390 | 1.00 | 33.74 |
| ATOM | 2860 | O | ARG | A | 356 | 62.746 | 22.732 | 110.950 | 1.00 | 34.68 |
| ATOM | 2861 | N | GLY | A | 357 | 64.361 | 24.181 | 111.550 | 1.00 | 35.60 |
| ATOM | 2862 | CA | GLY | A | 357 | 63.556 | 25.345 | 111.220 | 1.00 | 35.43 |
| ATOM | 2863 | C | GLY | A | 357 | 63.719 | 25.932 | 109.830 | 1.00 | 38.08 |
| ATOM | 2864 | O | GLY | A | 357 | 64.112 | 25.250 | 108.885 | 1.00 | 37.29 |
| ATOM | 2865 | N | GLY | A | 358 | 63.406 | 27.218 | 109.721 | 1.00 | 39.67 |
| ATOM | 2866 | CA | GLY | A | 358 | 63.493 | 27.925 | 108.457 | 1.00 | 36.36 |
| ATOM | 2867 | C | GLY | A | 358 | 62.398 | 28.966 | 108.499 | 1.00 | 39.45 |
| ATOM | 2868 | O | GLY | A | 358 | 61.763 | 29.131 | 109.539 | 1.00 | 37.58 |
| ATOM | 2869 | N | GLU | A | 359 | 62.163 | 29.662 | 107.391 | 1.00 | 40.89 |
| ATOM | 2870 | CA | GLU | A | 359 | 61.121 | 30.682 | 107.358 | 1.00 | 41.37 |
| ATOM | 2871 | CB | GLU | A | 359 | 61.310 | 31.627 | 106.172 | 1.00 | 44.64 |
| ATOM | 2872 | CG | GLU | A | 359 | 60.956 | 30.977 | 104.848 | 1.00 | 52.13 |
| ATOM | 2873 | CD | GLU | A | 359 | 60.833 | 31.973 | 103.708 | 1.00 | 59.14 |
| ATOM | 2874 | OE1 | GLU | A | 359 | 60.448 | 31.551 | 102.593 | 1.00 | 60.47 |
| ATOM | 2875 | OE2 | GLU | A | 359 | 61.119 | 33.173 | 103.923 | 1.00 | 57.77 |
| ATOM | 2876 | C | GLU | A | 359 | 59.770 | 30.006 | 107.200 | 1.00 | 38.02 |
| ATOM | 2877 | O | GLU | A | 359 | 59.689 | 28.828 | 106.850 | 1.00 | 35.29 |
| ATOM | 2878 | N | VAL | A | 360 | 58.708 | 30.762 | 107.441 | 1.00 | 36.81 |
| ATOM | 2879 | CA | VAL | A | 360 | 57.363 | 30.237 | 107.291 | 1.00 | 35.97 |
| ATOM | 2880 | CB | VAL | A | 360 | 56.401 | 30.789 | 108.368 | 1.00 | 34.90 |
| ATOM | 2881 | CG1 | VAL | A | 360 | 54.999 | 30.251 | 108.133 | 1.00 | 36.53 |
| ATOM | 2882 | CG2 | VAL | A | 360 | 56.888 | 30.393 | 109.755 | 1.00 | 37.06 |
| ATOM | 2883 | C | VAL | A | 360 | 56.886 | 30.690 | 105.928 | 1.00 | 36.74 |
| ATOM | 2884 | O | VAL | A | 360 | 56.661 | 31.881 | 105.712 | 1.00 | 34.90 |
| ATOM | 2885 | N | ARG | A | 361 | 56.753 | 29.741 | 105.004 | 1.00 | 35.48 |
| ATOM | 2886 | CA | ARG | A | 361 | 56.301 | 30.049 | 103.652 | 1.00 | 38.21 |
| ATOM | 2887 | CB | ARG | A | 361 | 56.152 | 28.776 | 102.815 | 1.00 | 39.76 |
| ATOM | 2888 | CG | ARG | A | 361 | 57.416 | 28.342 | 102.098 | 1.00 | 39.93 |
| ATOM | 2889 | CD | ARG | A | 361 | 57.225 | 26.963 | 101.486 | 1.00 | 38.68 |
| ATOM | 2890 | NE | ARG | A | 361 | 57.112 | 25.940 | 102.525 | 1.00 | 39.72 |
| ATOM | 2891 | CZ | ARG | A | 361 | 56.952 | 24.643 | 102.286 | 1.00 | 38.79 |
| ATOM | 2892 | NH1 | ARG | A | 361 | 56.881 | 24.200 | 101.036 | 1.00 | 32.40 |
| ATOM | 2893 | NH2 | ARG | A | 361 | 56.899 | 23.785 | 103.297 | 1.00 | 36.58 |
| ATOM | 2894 | C | ARG | A | 361 | 54.996 | 30.807 | 103.603 | 1.00 | 38.98 |
| ATOM | 2895 | O | ARG | A | 361 | 54.120 | 30.636 | 104.452 | 1.00 | 39.07 |
| ATOM | 2896 | N | LYS | A | 362 | 54.880 | 31.634 | 102.573 | 1.00 | 39.95 |
| ATOM | 2897 | CA | LYS | A | 362 | 53.709 | 32.459 | 102.339 | 1.00 | 42.73 |
| ATOM | 2898 | CB | LYS | A | 362 | 53.931 | 33.301 | 101.078 | 1.00 | 44.92 |
| ATOM | 2899 | CG | LYS | A | 362 | 54.995 | 34.390 | 101.219 | 1.00 | 55.45 |
| ATOM | 2900 | CD | LYS | A | 362 | 56.351 | 33.842 | 101.671 | 1.00 | 58.28 |
| ATOM | 2901 | CE | LYS | A | 362 | 56.907 | 32.809 | 100.697 | 1.00 | 57.04 |
| ATOM | 2902 | NZ | LYS | A | 362 | 58.224 | 32.283 | 101.151 | 1.00 | 58.75 |
| ATOM | 2903 | C | LYS | A | 362 | 52.434 | 31.634 | 102.200 | 1.00 | 40.51 |
| ATOM | 2904 | O | LYS | A | 362 | 51.391 | 31.996 | 102.748 | 1.00 | 36.10 |

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Figure 18-45

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|---------|------|-------|
| ATOM | 2905 | N | GLU A 363 | 52.506 | 30.527 | 101.469 | 1.00 | 37.79 |
| ATOM | 2906 | CA | GLU A 363 | 51.313 | 29.705 | 101.295 | 1.00 | 40.96 |
| ATOM | 2907 | CB | GLU A 363 | 51.587 | 28.530 | 100.347 | 1.00 | 43.62 |
| ATOM | 2908 | CG | GLU A 363 | 52.729 | 27.616 | 100.739 | 1.00 | 47.01 |
| ATOM | 2909 | CD | GLU A 363 | 52.995 | 26.547 | 99.683 | 1.00 | 51.65 |
| ATOM | 2910 | OE1 | GLU A 363 | 52.080 | 25.737 | 99.409 | 1.00 | 45.63 |
| ATOM | 2911 | OE2 | GLU A 363 | 54.116 | 26.526 | 99.125 | 1.00 | 48.44 |
| ATOM | 2912 | C | GLU A 363 | 50.788 | 29.209 | 102.636 | 1.00 | 37.74 |
| ATOM | 2913 | O | GLU A 363 | 49.582 | 29.113 | 102.834 | 1.00 | 34.79 |
| ATOM | 2914 | N | VAL A 364 | 51.691 | 28.910 | 103.564 | 1.00 | 33.64 |
| ATOM | 2915 | CA | VAL A 364 | 51.274 | 28.455 | 104.886 | 1.00 | 32.39 |
| ATOM | 2916 | CB | VAL A 364 | 52.484 | 28.048 | 105.749 | 1.00 | 33.99 |
| ATOM | 2917 | CG1 | VAL A 364 | 52.018 | 27.676 | 107.160 | 1.00 | 36.90 |
| ATOM | 2918 | CG2 | VAL A 364 | 53.198 | 26.867 | 105.109 | 1.00 | 29.56 |
| ATOM | 2919 | C | VAL A 364 | 50.506 | 29.574 | 105.589 | 1.00 | 34.33 |
| ATOM | 2920 | O | VAL A 364 | 49.454 | 29.336 | 106.188 | 1.00 | 29.80 |
| ATOM | 2921 | N | LYS A 365 | 51.027 | 30.797 | 105.499 | 1.00 | 38.12 |
| ATOM | 2922 | CA | LYS A 365 | 50.381 | 31.952 | 106.119 | 1.00 | 36.77 |
| ATOM | 2923 | CB | LYS A 365 | 51.255 | 33.204 | 105.969 | 1.00 | 37.98 |
| ATOM | 2924 | CG | LYS A 365 | 52.629 | 33.084 | 106.610 | 1.00 | 37.99 |
| ATOM | 2925 | CD | LYS A 365 | 53.449 | 34.357 | 106.429 | 1.00 | 35.50 |
| ATOM | 2926 | CE | LYS A 365 | 54.837 | 34.190 | 107.032 | 1.00 | 40.35 |
| ATOM | 2927 | NZ | LYS A 365 | 55.674 | 35.407 | 106.877 | 1.00 | 43.74 |
| ATOM | 2928 | C | LYS A 365 | 49.025 | 32.191 | 105.468 | 1.00 | 36.62 |
| ATOM | 2929 | O | LYS A 365 | 48.038 | 32.469 | 106.148 | 1.00 | 33.53 |
| ATOM | 2930 | N | ASP A 366 | 48.968 | 32.073 | 104.147 | 1.00 | 37.05 |
| ATOM | 2931 | CA | ASP A 366 | 47.708 | 32.278 | 103.449 | 1.00 | 37.72 |
| ATOM | 2932 | CB | ASP A 366 | 47.906 | 32.237 | 101.929 | 1.00 | 40.57 |
| ATOM | 2933 | CG | ASP A 366 | 48.833 | 33.334 | 101.427 | 1.00 | 43.98 |
| ATOM | 2934 | OD1 | ASP A 366 | 49.078 | 34.304 | 102.176 | 1.00 | 38.51 |
| ATOM | 2935 | OD2 | ASP A 366 | 49.297 | 33.235 | 100.269 | 1.00 | 41.96 |
| ATOM | 2936 | C | ASP A 366 | 46.670 | 31.238 | 103.862 | 1.00 | 39.24 |
| ATOM | 2937 | O | ASP A 366 | 45.497 | 31.562 | 104.029 | 1.00 | 39.04 |
| ATOM | 2938 | N | THR A 367 | 47.096 | 29.990 | 104.031 | 1.00 | 38.99 |
| ATOM | 2939 | CA | THR A 367 | 46.167 | 28.935 | 104.432 | 1.00 | 36.80 |
| ATOM | 2940 | CB | THR A 367 | 46.868 | 27.560 | 104.527 | 1.00 | 33.84 |
| ATOM | 2941 | OG1 | THR A 367 | 47.332 | 27.167 | 103.232 | 1.00 | 34.92 |
| ATOM | 2942 | CG2 | THR A 367 | 45.904 | 26.509 | 105.046 | 1.00 | 35.11 |
| ATOM | 2943 | C | THR A 367 | 45.532 | 29.257 | 105.786 | 1.00 | 36.58 |
| ATOM | 2944 | O | THR A 367 | 44.307 | 29.202 | 105.931 | 1.00 | 30.18 |
| ATOM | 2945 | N | LEU A 368 | 46.363 | 29.581 | 106.776 | 1.00 | 35.32 |
| ATOM | 2946 | CA | LEU A 368 | 45.850 | 29.926 | 108.095 | 1.00 | 35.46 |
| ATOM | 2947 | CB | LEU A 368 | 46.997 | 30.169 | 109.077 | 1.00 | 34.03 |
| ATOM | 2948 | CG | LEU A 368 | 47.545 | 28.925 | 109.794 | 1.00 | 39.04 |
| ATOM | 2949 | CD1 | LEU A 368 | 46.449 | 28.358 | 110.688 | 1.00 | 37.35 |
| ATOM | 2950 | CD2 | LEU A 368 | 48.014 | 27.871 | 108.797 | 1.00 | 39.52 |
| ATOM | 2951 | C | LEU A 368 | 44.957 | 31.156 | 107.994 | 1.00 | 38.12 |
| ATOM | 2952 | O | LEU A 368 | 43.968 | 31.277 | 108.719 | 1.00 | 31.70 |
| ATOM | 2953 | N | GLU A 369 | 45.307 | 32.063 | 107.086 | 1.00 | 40.45 |
| ATOM | 2954 | CA | GLU A 369 | 44.509 | 33.261 | 106.866 | 1.00 | 45.36 |
| ATOM | 2955 | CB | GLU A 369 | 45.128 | 34.126 | 105.765 | 1.00 | 47.38 |
| ATOM | 2956 | CG | GLU A 369 | 46.020 | 35.228 | 106.283 | 1.00 | 53.81 |
| ATOM | 2957 | CD | GLU A 369 | 45.227 | 36.306 | 106.996 | 1.00 | 59.97 |
| ATOM | 2958 | OE1 | GLU A 369 | 45.846 | 37.252 | 107.526 | 1.00 | 60.65 |
| ATOM | 2959 | OE2 | GLU A 369 | 43.980 | 36.211 | 107.016 | 1.00 | 63.69 |
| ATOM | 2960 | C | GLU A 369 | 43.100 | 32.865 | 106.466 | 1.00 | 43.23 |
| ATOM | 2961 | O | GLU A 369 | 42.130 | 33.283 | 107.095 | 1.00 | 44.62 |
| ATOM | 2962 | N | LYS A 370 | 42.983 | 32.057 | 105.417 | 1.00 | 40.34 |
| ATOM | 2963 | CA | LYS A 370 | 41.666 | 31.631 | 104.977 | 1.00 | 43.36 |
| ATOM | 2964 | CB | LYS A 370 | 41.738 | 30.773 | 103.704 | 1.00 | 44.79 |
| ATOM | 2965 | CG | LYS A 370 | 42.032 | 31.546 | 102.419 | 1.00 | 48.93 |
| ATOM | 2966 | CD | LYS A 370 | 43.503 | 31.514 | 102.019 | 1.00 | 51.41 |
| ATOM | 2967 | CE | LYS A 370 | 43.921 | 30.116 | 101.561 | 1.00 | 51.14 |
| ATOM | 2968 | NZ | LYS A 370 | 45.339 | 30.062 | 101.091 | 1.00 | 50.34 |
| ATOM | 2969 | C | LYS A 370 | 40.959 | 30.848 | 106.069 | 1.00 | 43.09 |
| ATOM | 2970 | O | LYS A 370 | 39.745 | 30.977 | 106.248 | 1.00 | 41.34 |

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Figure 18-46

| | | | | | | | | | |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 2971 | N | ALA A | 371 | 41.715 | 30.037 | 106.802 | 1.00 | 39.56 |
| ATOM | 2972 | CA | ALA A | 371 | 41.120 | 29.238 | 107.861 | 1.00 | 43.57 |
| ATOM | 2973 | CB | ALA A | 371 | 42.193 | 28.440 | 108.594 | 1.00 | 39.11 |
| ATOM | 2974 | C | ALA A | 371 | 40.365 | 30.132 | 108.837 | 1.00 | 46.10 |
| ATOM | 2975 | O | ALA A | 371 | 39.230 | 29.829 | 109.210 | 1.00 | 46.07 |
| ATOM | 2976 | N | LYS A | 372 | 40.981 | 31.239 | 109.227 | 1.00 | 46.62 |
| ATOM | 2977 | CA | LYS A | 372 | 40.391 | 32.178 | 110.192 | 1.00 | 48.18 |
| ATOM | 2978 | C | LYS A | 372 | 39.052 | 32.698 | 109.664 | 1.00 | 51.67 |
| ATOM | 2979 | O | LYS A | 372 | 38.294 | 33.318 | 110.432 | 1.00 | 53.21 |
| ATOM | 2980 | CB | LYS A | 372 | 41.334 | 33.364 | 110.413 | 1.00 | 47.22 |
| ATOM | 2981 | CG | LYS A | 372 | 42.804 | 32.949 | 110.510 | 1.00 | 20.00 |
| ATOM | 2982 | CD | LYS A | 372 | 43.746 | 34.131 | 110.752 | 1.00 | 20.00 |
| ATOM | 2983 | CE | LYS A | 372 | 45.216 | 33.715 | 110.849 | 1.00 | 20.00 |
| ATOM | 2984 | NZ | LYS A | 372 | 46.121 | 34.850 | 111.081 | 1.00 | 20.00 |
| ATOM | 2985 | N | ALA A | 373 | 38.751 | 32.476 | 108.397 | 1.00 | 57.71 |
| ATOM | 2986 | CA | ALA A | 373 | 37.492 | 32.933 | 107.806 | 1.00 | 58.67 |
| ATOM | 2987 | CB | ALA A | 373 | 37.758 | 33.632 | 106.480 | 1.00 | 57.19 |
| ATOM | 2988 | C | ALA A | 373 | 36.524 | 31.773 | 107.594 | 1.00 | 59.58 |
| ATOM | 2989 | O | ALA A | 373 | 35.432 | 31.797 | 108.205 | 1.00 | 60.89 |
| ATOM | 2990 | OXT | ALA A | 373 | 36.870 | 30.853 | 106.822 | 1.00 | 60.10 |
| ATOM | 3014 | CB | ALA B | 2 | 54.881 | -4.431 | 56.836 | 1.00 | 55.77 |
| ATOM | 3015 | C | ALA B | 2 | 53.960 | -2.137 | 56.480 | 1.00 | 57.58 |
| ATOM | 3016 | O | ALA B | 2 | 54.920 | -1.720 | 57.131 | 1.00 | 56.75 |
| ATOM | 3017 | N | ALA B | 2 | 54.263 | -3.672 | 54.557 | 1.00 | 58.22 |
| ATOM | 3018 | CA | ALA B | 2 | 53.914 | -3.584 | 56.008 | 1.00 | 58.47 |
| ATOM | 3019 | N | LYS B | 3 | 52.919 | -1.376 | 56.151 | 1.00 | 52.79 |
| ATOM | 3020 | CA | LYS B | 3 | 52.855 | 0.022 | 56.543 | 1.00 | 49.68 |
| ATOM | 3021 | CB | LYS B | 3 | 51.643 | 0.700 | 55.896 | 1.00 | 53.14 |
| ATOM | 3022 | CG | LYS B | 3 | 51.751 | 0.785 | 54.377 | 1.00 | 53.37 |
| ATOM | 3023 | CD | LYS B | 3 | 50.685 | 1.681 | 53.786 | 1.00 | 55.40 |
| ATOM | 3024 | CE | LYS B | 3 | 50.808 | 1.783 | 52.277 | 1.00 | 59.51 |
| ATOM | 3025 | NZ | LYS B | 3 | 52.140 | 2.323 | 51.884 | 1.00 | 56.88 |
| ATOM | 3026 | C | LYS B | 3 | 52.849 | 0.238 | 58.059 | 1.00 | 46.83 |
| ATOM | 3027 | O | LYS B | 3 | 52.389 | -0.607 | 58.830 | 1.00 | 41.63 |
| ATOM | 3028 | N | VAL B | 4 | 53.376 | 1.385 | 58.467 | 1.00 | 41.46 |
| ATOM | 3029 | CA | VAL B | 4 | 53.483 | 1.751 | 59.871 | 1.00 | 40.85 |
| ATOM | 3030 | CB | VAL B | 4 | 54.893 | 2.288 | 60.163 | 1.00 | 39.55 |
| ATOM | 3031 | CG1 | VAL B | 4 | 55.070 | 2.541 | 61.648 | 1.00 | 41.23 |
| ATOM | 3032 | CG2 | VAL B | 4 | 55.916 | 1.306 | 59.652 | 1.00 | 38.96 |
| ATOM | 3033 | C | VAL B | 4 | 52.451 | 2.813 | 60.230 | 1.00 | 38.92 |
| ATOM | 3034 | O | VAL B | 4 | 52.472 | 3.916 | 59.691 | 1.00 | 42.80 |
| ATOM | 3035 | N | LYS B | 5 | 51.559 | 2.479 | 61.157 | 1.00 | 34.90 |
| ATOM | 3036 | CA | LYS B | 5 | 50.501 | 3.396 | 61.558 | 1.00 | 31.22 |
| ATOM | 3037 | CB | LYS B | 5 | 49.133 | 2.796 | 61.215 | 1.00 | 33.76 |
| ATOM | 3038 | CG | LYS B | 5 | 48.841 | 2.623 | 59.726 | 1.00 | 36.60 |
| ATOM | 3039 | CD | LYS B | 5 | 48.667 | 3.964 | 59.032 | 1.00 | 41.48 |
| ATOM | 3040 | CE | LYS B | 5 | 48.234 | 3.803 | 57.577 | 1.00 | 43.62 |
| ATOM | 3041 | NZ | LYS B | 5 | 49.215 | 3.025 | 56.781 | 1.00 | 42.53 |
| ATOM | 3042 | C | LYS B | 5 | 50.512 | 3.749 | 63.038 | 1.00 | 32.67 |
| ATOM | 3043 | O | LYS B | 5 | 51.012 | 2.995 | 63.878 | 1.00 | 25.78 |
| ATOM | 3044 | N | LEU B | 6 | 49.937 | 4.906 | 63.343 | 1.00 | 27.07 |
| ATOM | 3045 | CA | LEU B | 6 | 49.821 | 5.379 | 64.712 | 1.00 | 31.09 |
| ATOM | 3046 | CB | LEU B | 6 | 50.596 | 6.696 | 64.896 | 1.00 | 30.13 |
| ATOM | 3047 | CG | LEU B | 6 | 50.691 | 7.340 | 66.285 | 1.00 | 28.09 |
| ATOM | 3048 | CD1 | LEU B | 6 | 49.333 | 7.827 | 66.728 | 1.00 | 38.87 |
| ATOM | 3049 | CD2 | LEU B | 6 | 51.248 | 6.338 | 67.282 | 1.00 | 24.87 |
| ATOM | 3050 | C | LEU B | 6 | 48.324 | 5.594 | 64.924 | 1.00 | 29.52 |
| ATOM | 3051 | O | LEU B | 6 | 47.669 | 6.287 | 64.149 | 1.00 | 33.36 |
| ATOM | 3052 | N | ILE B | 7 | 47.777 | 4.975 | 65.960 | 1.00 | 28.02 |
| ATOM | 3053 | CA | ILE B | 7 | 46.361 | 5.111 | 66.250 | 1.00 | 23.83 |
| ATOM | 3054 | CB | ILE B | 7 | 45.736 | 3.761 | 66.670 | 1.00 | 25.11 |
| ATOM | 3055 | CG2 | ILE B | 7 | 44.309 | 3.974 | 67.127 | 1.00 | 23.59 |
| ATOM | 3056 | CG1 | ILE B | 7 | 45.690 | 2.794 | 65.477 | 1.00 | 31.00 |
| ATOM | 3057 | CD1 | ILE B | 7 | 47.021 | 2.406 | 64.906 | 1.00 | 38.60 |
| ATOM | 3058 | C | ILE B | 7 | 46.179 | 6.130 | 67.363 | 1.00 | 26.49 |
| ATOM | 3059 | O | ILE B | 7 | 46.766 | 6.005 | 68.430 | 1.00 | 26.68 |

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Figure 18-47

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3060 | N | GLY | B | 8 | 45.372 | 7.151 | 67.106 | 1.00 | 29.51 |
| ATOM | 3061 | CA | GLY | B | 8 | 45.151 | 8.170 | 68.117 | 1.00 | 30.28 |
| ATOM | 3062 | C | GLY | B | 8 | 44.217 | 9.273 | 67.667 | 1.00 | 28.79 |
| ATOM | 3063 | O | GLY | B | 8 | 43.629 | 9.207 | 66.590 | 1.00 | 19.70 |
| ATOM | 3064 | N | THR | B | 9 | 44.088 | 10.291 | 68.509 | 1.00 | 26.46 |
| ATOM | 3065 | CA | THR | B | 9 | 43.234 | 11.438 | 68.238 | 1.00 | 29.37 |
| ATOM | 3066 | CB | THR | B | 9 | 41.748 | 11.064 | 68.311 | 1.00 | 32.64 |
| ATOM | 3067 | OG1 | THR | B | 9 | 40.959 | 12.253 | 68.218 | 1.00 | 30.35 |
| ATOM | 3068 | CG2 | THR | B | 9 | 41.431 | 10.383 | 69.637 | 1.00 | 33.42 |
| ATOM | 3069 | C | THR | B | 9 | 43.479 | 12.496 | 69.302 | 1.00 | 33.42 |
| ATOM | 3070 | O | THR | B | 9 | 43.884 | 12.173 | 70.416 | 1.00 | 30.46 |
| ATOM | 3071 | N | LEU | B | 10 | 43.228 | 13.754 | 68.961 | 1.00 | 32.05 |
| ATOM | 3072 | CA | LEU | B | 10 | 43.396 | 14.840 | 69.914 | 1.00 | 34.75 |
| ATOM | 3073 | CB | LEU | B | 10 | 43.381 | 16.189 | 69.190 | 1.00 | 38.02 |
| ATOM | 3074 | CG | LEU | B | 10 | 44.605 | 16.578 | 68.355 | 1.00 | 40.82 |
| ATOM | 3075 | CD1 | LEU | B | 10 | 44.961 | 15.472 | 67.394 | 1.00 | 43.62 |
| ATOM | 3076 | CD2 | LEU | B | 10 | 44.314 | 17.869 | 67.605 | 1.00 | 34.99 |
| ATOM | 3077 | C | LEU | B | 10 | 42.272 | 14.809 | 70.945 | 1.00 | 34.25 |
| ATOM | 3078 | O | LEU | B | 10 | 42.415 | 15.348 | 72.042 | 1.00 | 33.13 |
| ATOM | 3079 | N | ASP | B | 11 | 41.158 | 14.169 | 70.595 | 1.00 | 30.61 |
| ATOM | 3080 | CA | ASP | B | 11 | 40.011 | 14.098 | 71.501 | 1.00 | 33.08 |
| ATOM | 3081 | CB | ASP | B | 11 | 38.928 | 13.167 | 70.945 | 1.00 | 37.57 |
| ATOM | 3082 | CG | ASP | B | 11 | 38.372 | 13.643 | 69.621 | 1.00 | 43.14 |
| ATOM | 3083 | OD1 | ASP | B | 11 | 38.013 | 14.834 | 69.525 | 1.00 | 42.22 |
| ATOM | 3084 | OD2 | ASP | B | 11 | 38.281 | 12.825 | 68.681 | 1.00 | 45.58 |
| ATOM | 3085 | C | ASP | B | 11 | 40.358 | 13.654 | 72.919 | 1.00 | 32.19 |
| ATOM | 3086 | O | ASP | B | 11 | 39.688 | 14.053 | 73.875 | 1.00 | 23.44 |
| ATOM | 3087 | N | TYR | B | 12 | 41.386 | 12.822 | 73.066 | 1.00 | 28.02 |
| ATOM | 3088 | CA | TYR | B | 12 | 41.770 | 12.373 | 74.402 | 1.00 | 32.00 |
| ATOM | 3089 | CB | TYR | B | 12 | 43.011 | 11.476 | 74.363 | 1.00 | 28.67 |
| ATOM | 3090 | CG | TYR | B | 12 | 42.821 | 10.108 | 73.737 | 1.00 | 25.33 |
| ATOM | 3091 | CD1 | TYR | B | 12 | 43.338 | 9.823 | 72.475 | 1.00 | 23.74 |
| ATOM | 3092 | CE1 | TYR | B | 12 | 43.235 | 8.546 | 71.924 | 1.00 | 22.85 |
| ATOM | 3093 | CD2 | TYR | B | 12 | 42.183 | 9.077 | 74.436 | 1.00 | 21.93 |
| ATOM | 3094 | CE2 | TYR | B | 12 | 42.074 | 7.793 | 73.889 | 1.00 | 21.99 |
| ATOM | 3095 | CZ | TYR | B | 12 | 42.605 | 7.538 | 72.640 | 1.00 | 22.99 |
| ATOM | 3096 | OH | TYR | B | 12 | 42.532 | 6.273 | 72.109 | 1.00 | 18.79 |
| ATOM | 3097 | C | TYR | B | 12 | 42.054 | 13.567 | 75.319 | 1.00 | 32.74 |
| ATOM | 3098 | O | TYR | B | 12 | 41.986 | 13.450 | 76.542 | 1.00 | 23.85 |
| ATOM | 3099 | N | GLY | B | 13 | 42.374 | 14.710 | 74.720 | 1.00 | 26.96 |
| ATOM | 3100 | CA | GLY | B | 13 | 42.658 | 15.900 | 75.501 | 1.00 | 34.92 |
| ATOM | 3101 | C | GLY | B | 13 | 41.452 | 16.396 | 76.277 | 1.00 | 36.82 |
| ATOM | 3102 | O | GLY | B | 13 | 41.580 | 17.228 | 77.176 | 1.00 | 34.10 |
| ATOM | 3103 | N | LYS | B | 14 | 40.279 | 15.875 | 75.929 | 1.00 | 37.23 |
| ATOM | 3104 | CA | LYS | B | 14 | 39.031 | 16.247 | 76.584 | 1.00 | 41.77 |
| ATOM | 3105 | CB | LYS | B | 14 | 37.925 | 16.406 | 75.537 | 1.00 | 45.82 |
| ATOM | 3106 | CG | LYS | B | 14 | 38.110 | 17.585 | 74.579 | 1.00 | 51.38 |
| ATOM | 3107 | CD | LYS | B | 14 | 37.805 | 18.939 | 75.241 | 1.00 | 57.78 |
| ATOM | 3108 | CE | LYS | B | 14 | 38.752 | 19.285 | 76.388 | 1.00 | 58.82 |
| ATOM | 3109 | NZ | LYS | B | 14 | 38.387 | 20.568 | 77.070 | 1.00 | 55.06 |
| ATOM | 3110 | C | LYS | B | 14 | 38.591 | 15.226 | 77.627 | 1.00 | 39.50 |
| ATOM | 3111 | O | LYS | B | 14 | 37.546 | 15.385 | 78.252 | 1.00 | 35.54 |
| ATOM | 3112 | N | TYR | B | 15 | 39.395 | 14.186 | 77.815 | 1.00 | 40.97 |
| ATOM | 3113 | CA | TYR | B | 15 | 39.070 | 13.128 | 78.768 | 1.00 | 44.15 |
| ATOM | 3114 | CB | TYR | B | 15 | 38.863 | 11.827 | 77.990 | 1.00 | 44.42 |
| ATOM | 3115 | CG | TYR | B | 15 | 37.850 | 11.972 | 76.876 | 1.00 | 42.02 |
| ATOM | 3116 | CD1 | TYR | B | 15 | 38.064 | 11.389 | 75.634 | 1.00 | 41.06 |
| ATOM | 3117 | CE1 | TYR | B | 15 | 37.138 | 11.530 | 74.603 | 1.00 | 42.76 |
| ATOM | 3118 | CD2 | TYR | B | 15 | 36.678 | 12.703 | 77.065 | 1.00 | 42.99 |
| ATOM | 3119 | CE2 | TYR | B | 15 | 35.748 | 12.851 | 76.048 | 1.00 | 43.30 |
| ATOM | 3120 | CZ | TYR | B | 15 | 35.984 | 12.261 | 74.816 | 1.00 | 45.49 |
| ATOM | 3121 | OH | TYR | B | 15 | 35.066 | 12.403 | 73.801 | 1.00 | 45.69 |
| ATOM | 3122 | C | TYR | B | 15 | 40.151 | 12.944 | 79.838 | 1.00 | 43.48 |
| ATOM | 3123 | O | TYR | B | 15 | 40.519 | 11.819 | 80.167 | 1.00 | 41.20 |
| ATOM | 3124 | N | ARG | B | 16 | 40.647 | 14.052 | 80.381 | 1.00 | 43.01 |
| ATOM | 3125 | CA | ARG | B | 16 | 41.686 | 14.012 | 81.410 | 1.00 | 43.70 |

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Figure 18-48

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3126 | CB | ARG | B | 16 | 42.250 | 15.410 | 81.663 | 1.00 | 49.13 |
| ATOM | 3127 | CG | ARG | B | 16 | 42.656 | 16.197 | 80.447 | 1.00 | 54.22 |
| ATOM | 3128 | CD | ARG | B | 16 | 43.858 | 15.624 | 79.751 | 1.00 | 55.13 |
| ATOM | 3129 | NE | ARG | B | 16 | 44.303 | 16.549 | 78.718 | 1.00 | 62.87 |
| ATOM | 3130 | CZ | ARG | B | 16 | 44.628 | 17.818 | 78.951 | 1.00 | 64.92 |
| ATOM | 3131 | NH1 | ARG | B | 16 | 44.556 | 18.308 | 80.182 | 1.00 | 65.86 |
| ATOM | 3132 | NH2 | ARG | B | 16 | 45.022 | 18.600 | 77.954 | 1.00 | 67.15 |
| ATOM | 3133 | C | ARG | B | 16 | 41.093 | 13.531 | 82.728 | 1.00 | 42.97 |
| ATOM | 3134 | O | ARG | B | 16 | 39.882 | 13.593 | 82.927 | 1.00 | 38.44 |
| ATOM | 3135 | N | TYR | B | 17 | 41.949 | 13.056 | 83.628 | 1.00 | 39.36 |
| ATOM | 3136 | CA | TYR | B | 17 | 41.494 | 12.637 | 84.945 | 1.00 | 37.67 |
| ATOM | 3137 | CB | TYR | B | 17 | 42.500 | 11.679 | 85.584 | 1.00 | 31.69 |
| ATOM | 3138 | CG | TYR | B | 17 | 42.413 | 10.250 | 85.087 | 1.00 | 28.00 |
| ATOM | 3139 | CD1 | TYR | B | 17 | 42.530 | 9.944 | 83.732 | 1.00 | 22.89 |
| ATOM | 3140 | CE1 | TYR | B | 17 | 42.502 | 8.618 | 83.287 | 1.00 | 21.42 |
| ATOM | 3141 | CD2 | TYR | B | 17 | 42.258 | 9.196 | 85.984 | 1.00 | 24.67 |
| ATOM | 3142 | CE2 | TYR | B | 17 | 42.229 | 7.873 | 85.556 | 1.00 | 24.48 |
| ATOM | 3143 | CZ | TYR | B | 17 | 42.355 | 7.587 | 84.210 | 1.00 | 27.13 |
| ATOM | 3144 | OH | TYR | B | 17 | 42.371 | 6.271 | 83.796 | 1.00 | 19.94 |
| ATOM | 3145 | C | TYR | B | 17 | 41.377 | 13.927 | 85.765 | 1.00 | 38.94 |
| ATOM | 3146 | O | TYR | B | 17 | 41.947 | 14.951 | 85.391 | 1.00 | 39.65 |
| ATOM | 3147 | N | PRO | B | 18 | 40.647 | 13.893 | 86.891 | 1.00 | 41.27 |
| ATOM | 3148 | CD | PRO | B | 18 | 39.958 | 12.728 | 87.462 | 1.00 | 43.62 |
| ATOM | 3149 | CA | PRO | B | 18 | 40.448 | 15.058 | 87.762 | 1.00 | 45.33 |
| ATOM | 3150 | CB | PRO | B | 18 | 39.648 | 14.473 | 88.928 | 1.00 | 44.09 |
| ATOM | 3151 | CG | PRO | B | 18 | 40.096 | 13.015 | 88.933 | 1.00 | 49.22 |
| ATOM | 3152 | C | PRO | B | 18 | 41.702 | 15.809 | 88.221 | 1.00 | 45.86 |
| ATOM | 3153 | O | PRO | B | 18 | 42.789 | 15.244 | 88.317 | 1.00 | 45.44 |
| ATOM | 3154 | N | LYS | B | 19 | 41.506 | 17.095 | 88.507 | 1.00 | 48.42 |
| ATOM | 3155 | CA | LYS | B | 19 | 42.535 | 18.040 | 88.952 | 1.00 | 51.03 |
| ATOM | 3156 | CB | LYS | B | 19 | 41.873 | 19.122 | 89.814 | 1.00 | 56.35 |
| ATOM | 3157 | CG | LYS | B | 19 | 40.630 | 18.657 | 90.563 | 1.00 | 65.69 |
| ATOM | 3158 | CD | LYS | B | 19 | 40.894 | 17.441 | 91.423 | 1.00 | 68.96 |
| ATOM | 3159 | CE | LYS | B | 19 | 39.602 | 16.882 | 91.999 | 1.00 | 71.85 |
| ATOM | 3160 | NZ | LYS | B | 19 | 39.825 | 15.603 | 92.731 | 1.00 | 72.79 |
| ATOM | 3161 | C | LYS | B | 19 | 43.830 | 17.593 | 89.639 | 1.00 | 48.62 |
| ATOM | 3162 | O | LYS | B | 19 | 44.912 | 18.009 | 89.235 | 1.00 | 49.04 |
| ATOM | 3163 | N | ASN | B | 20 | 43.745 | 16.775 | 90.678 | 1.00 | 43.99 |
| ATOM | 3164 | CA | ASN | B | 20 | 44.957 | 16.356 | 91.375 | 1.00 | 43.86 |
| ATOM | 3165 | CB | ASN | B | 20 | 44.740 | 16.440 | 92.890 | 1.00 | 45.92 |
| ATOM | 3166 | CG | ASN | B | 20 | 44.418 | 17.848 | 93.355 | 1.00 | 49.44 |
| ATOM | 3167 | OD1 | ASN | B | 20 | 45.194 | 18.779 | 93.138 | 1.00 | 47.72 |
| ATOM | 3168 | ND2 | ASN | B | 20 | 43.268 | 18.011 | 93.999 | 1.00 | 49.42 |
| ATOM | 3169 | C | ASN | B | 20 | 45.460 | 14.960 | 91.008 | 1.00 | 39.49 |
| ATOM | 3170 | O | ASN | B | 20 | 46.496 | 14.521 | 91.494 | 1.00 | 38.24 |
| ATOM | 3171 | N | HIS | B | 21 | 44.729 | 14.274 | 90.140 | 1.00 | 36.93 |
| ATOM | 3172 | CA | HIS | B | 21 | 45.091 | 12.923 | 87.723 | 1.00 | 33.57 |
| ATOM | 3173 | CB | HIS | B | 21 | 43.948 | 12.299 | 87.924 | 1.00 | 28.67 |
| ATOM | 3174 | CG | HIS | B | 21 | 44.068 | 10.817 | 88.750 | 1.00 | 32.14 |
| ATOM | 3175 | CD2 | HIS | B | 21 | 44.779 | 10.076 | 87.867 | 1.00 | 26.15 |
| ATOM | 3176 | ND1 | HIS | B | 21 | 43.431 | 9.917 | 89.578 | 1.00 | 29.59 |
| ATOM | 3177 | CE1 | HIS | B | 21 | 43.743 | 8.686 | 89.212 | 1.00 | 23.65 |
| ATOM | 3178 | NE2 | HIS | B | 21 | 44.560 | 8.755 | 88.177 | 1.00 | 29.71 |
| ATOM | 3179 | C | HIS | B | 21 | 46.348 | 12.928 | 88.852 | 1.00 | 29.06 |
| ATOM | 3180 | O | HIS | B | 21 | 46.536 | 13.805 | 88.015 | 1.00 | 24.86 |
| ATOM | 3181 | N | PRO | B | 22 | 47.225 | 11.937 | 89.035 | 1.00 | 30.50 |
| ATOM | 3182 | CD | PRO | B | 22 | 47.187 | 10.802 | 89.976 | 1.00 | 31.51 |
| ATOM | 3183 | CA | PRO | B | 22 | 48.446 | 11.880 | 88.231 | 1.00 | 29.58 |
| ATOM | 3184 | CB | PRO | B | 22 | 49.055 | 10.549 | 88.656 | 1.00 | 33.72 |
| ATOM | 3185 | CG | PRO | B | 22 | 43.658 | 10.489 | 90.124 | 1.00 | 31.07 |
| ATOM | 3186 | C | PRO | B | 22 | 48.176 | 11.950 | 86.728 | 1.00 | 28.52 |
| ATOM | 3187 | O | PRO | B | 22 | 48.989 | 12.474 | 85.972 | 1.00 | 31.85 |
| ATOM | 3188 | N | LEU | B | 23 | 47.030 | 11.435 | 86.297 | 1.00 | 24.47 |
| ATOM | 3189 | CA | LEU | B | 23 | 46.685 | 11.434 | 84.874 | 1.00 | 27.80 |
| ATOM | 3190 | CB | LEU | B | 23 | 45.933 | 10.141 | 84.513 | 1.00 | 22.18 |
| ATOM | 3191 | CG | LEU | B | 23 | 46.760 | 8.852 | 84.556 | 1.00 | 29.32 |

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Figure 18-49

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3192 | CD1 | LEU | B | 23 | 45.868 | 7.628 | 84.402 | 1.00 | 24.94 |
| ATOM | 3193 | CD2 | LEU | B | 23 | 47.805 | 8.905 | 83.446 | 1.00 | 24.80 |
| ATOM | 3194 | C | LEU | B | 23 | 45.891 | 12.638 | 84.367 | 1.00 | 27.95 |
| ATOM | 3195 | O | LEU | B | 23 | 45.166 | 12.528 | 83.373 | 1.00 | 24.42 |
| ATOM | 3196 | N | LYS | B | 24 | 46.011 | 13.793 | 85.018 | 1.00 | 31.01 |
| ATOM | 3197 | CA | LYS | B | 24 | 45.261 | 14.946 | 84.530 | 1.00 | 29.40 |
| ATOM | 3198 | CB | LYS | B | 24 | 44.934 | 15.923 | 85.665 | 1.00 | 33.03 |
| ATOM | 3199 | CG | LYS | B | 24 | 45.979 | 16.969 | 85.999 | 1.00 | 33.54 |
| ATOM | 3200 | CD | LYS | B | 24 | 47.300 | 16.397 | 86.422 | 1.00 | 39.10 |
| ATOM | 3201 | CE | LYS | B | 24 | 48.109 | 17.466 | 87.152 | 1.00 | 45.49 |
| ATOM | 3202 | NZ | LYS | B | 24 | 48.224 | 18.737 | 86.380 | 1.00 | 45.95 |
| ATOM | 3203 | C | LYS | B | 24 | 46.039 | 15.653 | 83.425 | 1.00 | 30.02 |
| ATOM | 3204 | O | LYS | B | 24 | 45.508 | 16.523 | 82.736 | 1.00 | 28.82 |
| ATOM | 3205 | N | ILE | B | 25 | 47.298 | 15.262 | 83.246 | 1.00 | 25.93 |
| ATOM | 3206 | CA | ILE | B | 25 | 48.139 | 15.858 | 82.212 | 1.00 | 29.48 |
| ATOM | 3207 | CB | ILE | B | 25 | 49.641 | 15.528 | 82.409 | 1.00 | 33.61 |
| ATOM | 3208 | CG2 | ILE | B | 25 | 50.126 | 16.033 | 83.775 | 1.00 | 32.27 |
| ATOM | 3209 | CG1 | ILE | B | 25 | 49.851 | 14.014 | 82.263 | 1.00 | 28.17 |
| ATOM | 3210 | CD1 | ILE | B | 25 | 51.310 | 13.584 | 82.188 | 1.00 | 36.32 |
| ATOM | 3211 | C | ILE | B | 25 | 47.784 | 15.318 | 80.834 | 1.00 | 30.08 |
| ATOM | 3212 | O | ILE | B | 25 | 47.263 | 14.210 | 80.704 | 1.00 | 25.37 |
| ATOM | 3213 | N | PRO | B | 26 | 48.064 | 16.101 | 79.783 | 1.00 | 29.19 |
| ATOM | 3214 | CD | PRO | B | 26 | 48.650 | 17.448 | 79.770 | 1.00 | 32.47 |
| ATOM | 3215 | CA | PRO | B | 26 | 47.782 | 15.673 | 78.413 | 1.00 | 29.52 |
| ATOM | 3216 | CB | PRO | B | 26 | 48.103 | 16.921 | 77.593 | 1.00 | 29.84 |
| ATOM | 3217 | CG | PRO | B | 26 | 47.930 | 18.046 | 78.599 | 1.00 | 36.40 |
| ATOM | 3218 | C | PRO | B | 26 | 48.789 | 14.561 | 78.137 | 1.00 | 27.64 |
| ATOM | 3219 | O | PRO | B | 26 | 49.920 | 14.620 | 78.629 | 1.00 | 23.08 |
| ATOM | 3220 | N | ARG | B | 27 | 48.403 | 13.557 | 77.360 | 1.00 | 23.09 |
| ATOM | 3221 | CA | ARG | B | 27 | 49.326 | 12.469 | 77.072 | 1.00 | 23.00 |
| ATOM | 3222 | CB | ARG | B | 27 | 48.987 | 11.264 | 77.962 | 1.00 | 26.21 |
| ATOM | 3223 | CG | ARG | B | 27 | 49.101 | 11.617 | 79.449 | 1.00 | 17.03 |
| ATOM | 3224 | CD | ARG | B | 27 | 48.663 | 10.507 | 80.416 | 1.00 | 26.83 |
| ATOM | 3225 | NE | ARG | B | 27 | 49.586 | 9.375 | 80.502 | 1.00 | 22.99 |
| ATOM | 3226 | CZ | ARG | B | 27 | 49.444 | 8.220 | 79.856 | 1.00 | 25.06 |
| ATOM | 3227 | NH1 | ARG | B | 27 | 48.408 | 8.022 | 79.059 | 1.00 | 17.74 |
| ATOM | 3228 | NH2 | ARG | B | 27 | 50.336 | 7.253 | 80.027 | 1.00 | 23.38 |
| ATOM | 3229 | C | ARG | B | 27 | 49.329 | 12.097 | 75.595 | 1.00 | 22.54 |
| ATOM | 3230 | O | ARG | B | 27 | 50.214 | 12.526 | 74.852 | 1.00 | 21.86 |
| ATOM | 3231 | N | VAL | B | 28 | 48.352 | 11.318 | 75.148 | 1.00 | 20.64 |
| ATOM | 3232 | CA | VAL | B | 28 | 48.337 | 10.954 | 73.739 | 1.00 | 26.57 |
| ATOM | 3233 | CB | VAL | B | 28 | 47.242 | 9.917 | 73.424 | 1.00 | 30.92 |
| ATOM | 3234 | CG1 | VAL | B | 28 | 47.195 | 9.645 | 71.925 | 1.00 | 27.04 |
| ATOM | 3235 | CG2 | VAL | B | 28 | 47.535 | 8.616 | 74.172 | 1.00 | 25.45 |
| ATOM | 3236 | C | VAL | B | 28 | 48.150 | 12.189 | 72.866 | 1.00 | 28.02 |
| ATOM | 3237 | O | VAL | B | 28 | 48.780 | 12.311 | 71.808 | 1.00 | 30.88 |
| ATOM | 3238 | N | SER | B | 29 | 47.298 | 13.112 | 73.304 | 1.00 | 24.30 |
| ATOM | 3239 | CA | SER | B | 29 | 47.082 | 14.326 | 72.523 | 1.00 | 29.48 |
| ATOM | 3240 | CB | SER | B | 29 | 45.939 | 15.169 | 73.110 | 1.00 | 31.72 |
| ATOM | 3241 | OG | SER | B | 29 | 46.218 | 15.614 | 74.424 | 1.00 | 34.55 |
| ATOM | 3242 | C | SER | B | 29 | 48.379 | 15.125 | 72.514 | 1.00 | 30.81 |
| ATOM | 3243 | O | SER | B | 29 | 48.680 | 15.820 | 71.545 | 1.00 | 28.85 |
| ATOM | 3244 | N | LEU | B | 30 | 49.157 | 15.003 | 73.589 | 1.00 | 29.63 |
| ATOM | 3245 | CA | LEU | B | 30 | 50.427 | 15.721 | 73.679 | 1.00 | 31.59 |
| ATOM | 3246 | CB | LEU | B | 30 | 51.046 | 15.593 | 75.079 | 1.00 | 29.49 |
| ATOM | 3247 | CG | LEU | B | 30 | 52.066 | 16.660 | 75.513 | 1.00 | 34.37 |
| ATOM | 3248 | CD1 | LEU | B | 30 | 52.937 | 16.083 | 76.610 | 1.00 | 30.15 |
| ATOM | 3249 | CD2 | LEU | B | 30 | 52.951 | 17.098 | 74.357 | 1.00 | 32.90 |
| ATOM | 3250 | C | LEU | B | 30 | 51.371 | 15.085 | 72.672 | 1.00 | 25.90 |
| ATOM | 3251 | O | LEU | B | 30 | 52.052 | 15.777 | 71.913 | 1.00 | 25.10 |
| ATOM | 3252 | N | LEU | B | 31 | 51.404 | 13.756 | 72.675 | 1.00 | 22.10 |
| ATOM | 3253 | CA | LEU | B | 31 | 52.268 | 13.013 | 71.764 | 1.00 | 25.52 |
| ATOM | 3254 | CB | LEU | B | 31 | 51.966 | 11.514 | 71.842 | 1.00 | 26.41 |
| ATOM | 3255 | CG | LEU | B | 31 | 53.066 | 10.524 | 71.441 | 1.00 | 28.93 |
| ATOM | 3256 | CD1 | LEU | B | 31 | 52.425 | 9.198 | 71.042 | 1.00 | 23.69 |
| ATOM | 3257 | CD2 | LEU | B | 31 | 53.873 | 11.049 | 70.300 | 1.00 | 30.41 |

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Figure 18-50

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3258 | C | LEU | B | 31 | 52.010 | 13.489 | 70.335 | 1.00 | 25.38 |
| ATOM | 3259 | O | LEU | B | 31 | 52.940 | 13.851 | 69.614 | 1.00 | 21.03 |
| ATOM | 3260 | N | LEU | B | 32 | 50.741 | 13.481 | 69.933 | 1.00 | 21.27 |
| ATOM | 3261 | CA | LEU | B | 32 | 50.364 | 13.899 | 68.585 | 1.00 | 27.91 |
| ATOM | 3262 | CB | LEU | B | 32 | 48.841 | 13.798 | 68.408 | 1.00 | 26.60 |
| ATOM | 3263 | CG | LEU | B | 32 | 48.195 | 12.419 | 68.614 | 1.00 | 27.30 |
| ATOM | 3264 | CD1 | LEU | B | 32 | 46.699 | 12.504 | 68.321 | 1.00 | 31.60 |
| ATOM | 3265 | CD2 | LEU | B | 32 | 48.837 | 11.391 | 67.708 | 1.00 | 26.90 |
| ATOM | 3266 | C | LEU | B | 32 | 50.835 | 15.317 | 68.242 | 1.00 | 26.07 |
| ATOM | 3267 | O | LEU | B | 32 | 51.458 | 15.533 | 67.205 | 1.00 | 22.45 |
| ATOM | 3268 | N | ARG | B | 33 | 50.545 | 16.282 | 69.111 | 1.00 | 28.19 |
| ATOM | 3269 | CA | ARG | B | 33 | 50.962 | 17.660 | 68.865 | 1.00 | 31.77 |
| ATOM | 3270 | CB | ARG | B | 33 | 50.395 | 18.601 | 69.930 | 1.00 | 34.22 |
| ATOM | 3271 | CG | ARG | B | 33 | 48.887 | 18.740 | 69.904 | 1.00 | 40.33 |
| ATOM | 3272 | CD | ARG | B | 33 | 48.420 | 19.713 | 70.970 | 1.00 | 47.67 |
| ATOM | 3273 | NE | ARG | B | 33 | 46.977 | 19.931 | 70.924 | 1.00 | 56.24 |
| ATOM | 3274 | CZ | ARG | B | 33 | 46.330 | 20.505 | 69.912 | 1.00 | 60.10 |
| ATOM | 3275 | NH1 | ARG | B | 33 | 46.997 | 20.929 | 68.845 | 1.00 | 63.11 |
| ATOM | 3276 | NH2 | ARG | B | 33 | 45.011 | 20.652 | 69.965 | 1.00 | 63.81 |
| ATOM | 3277 | C | ARG | B | 33 | 52.476 | 17.791 | 68.852 | 1.00 | 30.12 |
| ATOM | 3278 | O | ARG | B | 33 | 53.028 | 18.580 | 68.097 | 1.00 | 30.20 |
| ATOM | 3279 | N | PHE | B | 34 | 53.147 | 17.012 | 69.694 | 1.00 | 30.70 |
| ATOM | 3280 | CA | PHE | B | 34 | 54.600 | 17.060 | 69.774 | 1.00 | 29.42 |
| ATOM | 3281 | CB | PHE | B | 34 | 55.096 | 16.176 | 70.920 | 1.00 | 30.46 |
| ATOM | 3282 | CG | PHE | B | 34 | 56.556 | 16.358 | 71.248 | 1.00 | 28.56 |
| ATOM | 3283 | CD1 | PHE | B | 34 | 57.001 | 17.515 | 71.885 | 1.00 | 26.92 |
| ATOM | 3284 | CD2 | PHE | B | 34 | 57.481 | 15.373 | 70.932 | 1.00 | 28.88 |
| ATOM | 3285 | CE1 | PHE | B | 34 | 58.346 | 17.684 | 72.206 | 1.00 | 28.15 |
| ATOM | 3286 | CE2 | PHE | B | 34 | 58.831 | 15.530 | 71.246 | 1.00 | 31.47 |
| ATOM | 3287 | CZ | PHE | B | 34 | 59.265 | 16.689 | 71.887 | 1.00 | 28.15 |
| ATOM | 3288 | C | PHE | B | 34 | 55.202 | 16.583 | 68.460 | 1.00 | 33.78 |
| ATOM | 3289 | O | PHE | B | 34 | 56.049 | 17.259 | 67.873 | 1.00 | 33.71 |
| ATOM | 3290 | N | LYS | B | 35 | 54.770 | 15.413 | 67.999 | 1.00 | 28.65 |
| ATOM | 3291 | CA | LYS | B | 35 | 55.294 | 14.880 | 66.753 | 1.00 | 34.33 |
| ATOM | 3292 | CB | LYS | B | 35 | 54.684 | 13.509 | 66.454 | 1.00 | 32.97 |
| ATOM | 3293 | CG | LYS | B | 35 | 55.141 | 12.423 | 67.414 | 1.00 | 34.93 |
| ATOM | 3294 | CD | LYS | B | 35 | 54.580 | 11.066 | 67.047 | 1.00 | 41.43 |
| ATOM | 3295 | CE | LYS | B | 35 | 53.070 | 11.004 | 67.205 | 1.00 | 44.04 |
| ATOM | 3296 | NZ | LYS | B | 35 | 52.335 | 11.984 | 66.345 | 1.00 | 60.09 |
| ATOM | 3297 | C | LYS | B | 35 | 55.015 | 15.842 | 65.608 | 1.00 | 35.78 |
| ATOM | 3298 | O | LYS | B | 35 | 55.869 | 16.061 | 64.752 | 1.00 | 33.39 |
| ATOM | 3299 | N | ASP | B | 36 | 53.823 | 16.426 | 65.602 | 1.00 | 32.32 |
| ATOM | 3300 | CA | ASP | B | 36 | 53.468 | 17.365 | 64.552 | 1.00 | 36.31 |
| ATOM | 3301 | CB | ASP | B | 36 | 52.015 | 17.800 | 64.698 | 1.00 | 42.56 |
| ATOM | 3302 | CG | ASP | B | 36 | 51.617 | 18.822 | 63.661 | 1.00 | 43.03 |
| ATOM | 3303 | OD1 | ASP | B | 36 | 51.812 | 18.544 | 62.461 | 1.00 | 39.17 |
| ATOM | 3304 | OD2 | ASP | B | 36 | 51.111 | 19.897 | 64.043 | 1.00 | 44.34 |
| ATOM | 3305 | C | ASP | B | 36 | 54.371 | 18.590 | 64.578 | 1.00 | 36.14 |
| ATOM | 3306 | O | ASP | B | 36 | 54.764 | 19.099 | 63.534 | 1.00 | 32.40 |
| ATOM | 3307 | N | ALA | B | 37 | 54.694 | 19.061 | 65.777 | 1.00 | 34.80 |
| ATOM | 3308 | CA | ALA | B | 37 | 55.554 | 20.226 | 65.924 | 1.00 | 36.82 |
| ATOM | 3309 | CB | ALA | B | 37 | 55.599 | 20.659 | 67.383 | 1.00 | 38.54 |
| ATOM | 3310 | C | ALA | B | 37 | 56.959 | 19.901 | 65.429 | 1.00 | 37.66 |
| ATOM | 3311 | O | ALA | B | 37 | 57.675 | 20.776 | 64.950 | 1.00 | 30.56 |
| ATOM | 3312 | N | MET | B | 38 | 57.346 | 18.635 | 65.541 | 1.00 | 37.42 |
| ATOM | 3313 | CA | MET | B | 38 | 58.670 | 18.192 | 65.107 | 1.00 | 36.25 |
| ATOM | 3314 | CB | MET | B | 38 | 59.158 | 17.059 | 66.013 | 1.00 | 36.44 |
| ATOM | 3315 | CG | MET | B | 38 | 59.341 | 17.438 | 67.474 | 1.00 | 37.68 |
| ATOM | 3316 | SD | MET | B | 38 | 60.841 | 18.391 | 67.784 | 1.00 | 38.07 |
| ATOM | 3317 | CE | MET | B | 38 | 62.093 | 17.228 | 67.300 | 1.00 | 30.98 |
| ATOM | 3318 | C | MET | B | 38 | 58.639 | 17.690 | 63.663 | 1.00 | 35.86 |
| ATOM | 3319 | O | MET | B | 38 | 59.659 | 17.262 | 63.130 | 1.00 | 32.69 |
| ATOM | 3320 | N | ASN | B | 39 | 57.470 | 17.742 | 63.035 | 1.00 | 35.82 |
| ATOM | 3321 | CA | ASN | B | 39 | 57.321 | 17.262 | 61.661 | 1.00 | 42.75 |
| ATOM | 3322 | CB | ASN | B | 39 | 58.156 | 18.108 | 60.688 | 1.00 | 46.20 |
| ATOM | 3323 | CG | ASN | B | 39 | 57.670 | 19.543 | 60.591 | 1.00 | 47.57 |

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Figure 18-51

| | | | | | | | | |
|------|------|-----------|----|--------|--------|--------|------|-------|
| ATOM | 3324 | OD1 ASN B | 39 | 56.524 | 19.801 | 60.212 | 1.00 | 48.78 |
| ATOM | 3325 | ND2 ASN B | 39 | 58.540 | 20.486 | 60.933 | 1.00 | 46.52 |
| ATOM | 3326 | C ASN B | 39 | 57.759 | 15.804 | 61.569 | 1.00 | 39.12 |
| ATOM | 3327 | O ASN B | 39 | 58.465 | 15.416 | 60.639 | 1.00 | 35.75 |
| ATOM | 3328 | N LEU B | 40 | 57.332 | 14.997 | 62.535 | 1.00 | 34.64 |
| ATOM | 3329 | CA LEU B | 40 | 57.700 | 13.590 | 62.556 | 1.00 | 35.10 |
| ATOM | 3330 | CB LEU B | 40 | 58.347 | 13.248 | 63.898 | 1.00 | 35.97 |
| ATOM | 3331 | CG LEU B | 40 | 59.595 | 14.073 | 64.227 | 1.00 | 36.21 |
| ATOM | 3332 | CD1 LEU B | 40 | 60.148 | 13.648 | 65.573 | 1.00 | 36.57 |
| ATOM | 3333 | CD2-LEU B | 40 | 60.646 | 13.880 | 63.145 | 1.00 | 36.79 |
| ATOM | 3334 | C LEU B | 40 | 56.549 | 12.626 | 62.264 | 1.00 | 37.58 |
| ATOM | 3335 | O LEU B | 40 | 56.637 | 11.438 | 62.573 | 1.00 | 39.15 |
| ATOM | 3336 | N ILE B | 41 | 55.476 | 13.131 | 61.663 | 1.00 | 36.79 |
| ATOM | 3337 | CA ILE B | 41 | 54.340 | 12.290 | 61.314 | 1.00 | 35.42 |
| ATOM | 3338 | CB ILE B | 41 | 53.445 | 11.991 | 62.536 | 1.00 | 35.21 |
| ATOM | 3339 | CG2 ILE B | 41 | 52.793 | 13.271 | 63.047 | 1.00 | 31.89 |
| ATOM | 3340 | CG1 ILE B | 41 | 52.367 | 10.980 | 62.141 | 1.00 | 32.68 |
| ATOM | 3341 | CD1 ILE B | 41 | 51.470 | 10.550 | 63.285 | 1.00 | 36.46 |
| ATOM | 3342 | C ILE B | 41 | 53.492 | 12.937 | 60.229 | 1.00 | 37.52 |
| ATOM | 3343 | O ILE B | 41 | 53.352 | 14.157 | 60.183 | 1.00 | 40.24 |
| ATOM | 3344 | N ASP B | 42 | 52.943 | 12.114 | 59.345 | 1.00 | 39.55 |
| ATOM | 3345 | CA ASP B | 42 | 52.094 | 12.615 | 58.273 | 1.00 | 45.30 |
| ATOM | 3346 | CB ASP B | 42 | 52.569 | 12.119 | 56.901 | 1.00 | 45.93 |
| ATOM | 3347 | CG ASP B | 42 | 53.972 | 12.584 | 56.564 | 1.00 | 47.09 |
| ATOM | 3348 | OD1 ASP B | 42 | 54.244 | 13.799 | 56.686 | 1.00 | 46.60 |
| ATOM | 3349 | OD2 ASP B | 42 | 54.797 | 11.736 | 56.162 | 1.00 | 45.16 |
| ATOM | 3350 | C ASP B | 42 | 50.677 | 12.134 | 58.524 | 1.00 | 45.15 |
| ATOM | 3351 | O ASP B | 42 | 50.467 | 11.051 | 59.069 | 1.00 | 47.06 |
| ATOM | 3352 | N GLU B | 43 | 49.707 | 12.944 | 58.121 | 1.00 | 48.13 |
| ATOM | 3353 | CA GLU B | 43 | 48.303 | 12.618 | 58.312 | 1.00 | 50.50 |
| ATOM | 3354 | CB GLU B | 43 | 47.441 | 13.637 | 57.571 | 1.00 | 53.54 |
| ATOM | 3355 | CG GLU B | 43 | 45.961 | 13.505 | 57.840 | 1.00 | 59.52 |
| ATOM | 3356 | CD GLU B | 43 | 45.155 | 14.518 | 57.065 | 1.00 | 64.03 |
| ATOM | 3357 | OE1 GLU B | 43 | 43.914 | 14.535 | 57.215 | 1.00 | 68.54 |
| ATOM | 3358 | OE2 GLU B | 43 | 45.765 | 15.298 | 56.301 | 1.00 | 66.95 |
| ATOM | 3359 | C GLU B | 43 | 47.972 | 11.205 | 57.836 | 1.00 | 47.81 |
| ATOM | 3360 | O GLU B | 43 | 47.092 | 10.547 | 58.390 | 1.00 | 49.67 |
| ATOM | 3361 | N LYS B | 44 | 48.690 | 10.744 | 56.817 | 1.00 | 46.21 |
| ATOM | 3362 | CA LYS B | 44 | 48.484 | 9.409 | 56.251 | 1.00 | 48.28 |
| ATOM | 3363 | CB LYS B | 44 | 49.207 | 9.311 | 54.894 | 1.00 | 49.96 |
| ATOM | 3364 | CG LYS B | 44 | 49.639 | 7.903 | 54.470 | 1.00 | 52.18 |
| ATOM | 3365 | CD LYS B | 44 | 50.970 | 7.532 | 55.127 | 1.00 | 61.03 |
| ATOM | 3366 | CE LYS B | 44 | 51.399 | 6.095 | 54.844 | 1.00 | 62.80 |
| ATOM | 3367 | NZ LYS B | 44 | 50.511 | 5.098 | 55.510 | 1.00 | 65.34 |
| ATOM | 3368 | C LYS B | 44 | 48.899 | 8.249 | 57.161 | 1.00 | 45.92 |
| ATOM | 3369 | O LYS B | 44 | 48.418 | 7.127 | 57.009 | 1.00 | 41.30 |
| ATOM | 3370 | N GLU B | 45 | 49.797 | 8.517 | 58.100 | 1.00 | 42.18 |
| ATOM | 3371 | CA GLU B | 45 | 50.268 | 7.486 | 59.014 | 1.00 | 38.41 |
| ATOM | 3372 | CB GLU B | 45 | 51.684 | 7.812 | 59.468 | 1.00 | 33.73 |
| ATOM | 3373 | CG GLU B | 45 | 52.694 | 7.887 | 58.351 | 1.00 | 37.58 |
| ATOM | 3374 | CD GLU B | 45 | 53.998 | 8.504 | 58.813 | 1.00 | 34.34 |
| ATOM | 3375 | OE1 GLU B | 45 | 53.997 | 9.699 | 59.176 | 1.00 | 38.04 |
| ATOM | 3376 | OE2 GLU B | 45 | 55.020 | 7.799 | 58.821 | 1.00 | 33.37 |
| ATOM | 3377 | C GLU B | 45 | 49.368 | 7.403 | 60.238 | 1.00 | 36.86 |
| ATOM | 3378 | O GLU B | 45 | 49.461 | 6.462 | 61.032 | 1.00 | 34.98 |
| ATOM | 3379 | N LEU B | 46 | 48.489 | 8.386 | 60.386 | 1.00 | 30.86 |
| ATOM | 3380 | CA LEU B | 46 | 47.608 | 8.438 | 61.545 | 1.00 | 30.65 |
| ATOM | 3381 | CB LEU B | 46 | 47.501 | 9.889 | 62.019 | 1.00 | 32.74 |
| ATOM | 3382 | CG LEU B | 46 | 46.642 | 10.163 | 63.250 | 1.00 | 34.76 |
| ATOM | 3383 | CD1 LEU B | 46 | 47.189 | 9.379 | 64.425 | 1.00 | 32.24 |
| ATOM | 3384 | CD2 LEU B | 46 | 46.639 | 11.656 | 63.548 | 1.00 | 33.94 |
| ATOM | 3385 | C LEU B | 46 | 46.212 | 7.861 | 61.318 | 1.00 | 31.36 |
| ATOM | 3386 | O LEU B | 46 | 45.530 | 8.218 | 60.363 | 1.00 | 31.78 |
| ATOM | 3387 | N ILE B | 47 | 45.801 | 6.957 | 62.203 | 1.00 | 31.18 |
| ATOM | 3388 | CA ILE B | 47 | 44.479 | 6.338 | 62.139 | 1.00 | 29.36 |
| ATOM | 3389 | CB ILE B | 47 | 44.564 | 4.802 | 62.258 | 1.00 | 28.62 |

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Figure 18-52

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3390 | CG2 | ILE | B | 47 | 43.161 | 4.205 | 62.407 | 1.00 | 28.80 |
| ATOM | 3391 | CG1 | ILE | B | 47 | 45.266 | 4.230 | 61.028 | 1.00 | 29.42 |
| ATOM | 3392 | CD1 | ILE | B | 47 | 45.419 | 2.722 | 61.054 | 1.00 | 31.12 |
| ATOM | 3393 | C | ILE | B | 47 | 43.659 | 6.875 | 63.303 | 1.00 | 32.22 |
| ATOM | 3394 | O | ILE | B | 47 | 44.063 | 6.755 | 64.461 | 1.00 | 31.17 |
| ATOM | 3395 | N | LYS | B | 48 | 42.514 | 7.475 | 62.999 | 1.00 | 28.39 |
| ATOM | 3396 | CA | LYS | B | 48 | 41.662 | 8.037 | 64.040 | 1.00 | 32.37 |
| ATOM | 3397 | CB | LYS | B | 48 | 40.517 | 8.840 | 63.414 | 1.00 | 36.32 |
| ATOM | 3398 | CG | LYS | B | 48 | 39.607 | 9.514 | 64.430 | 1.00 | 43.08 |
| ATOM | 3399 | CD | LYS | B | 48 | 38.535 | 10.361 | 63.747 | 1.00 | 44.38 |
| ATOM | 3400 | CE | LYS | B | 48 | 37.657 | 11.074 | 64.768 | 1.00 | 45.91 |
| ATOM | 3401 | NZ | LYS | B | 48 | 38.451 | 11.991 | 65.643 | 1.00 | 42.66 |
| ATOM | 3402 | C | LYS | B | 48 | 41.095 | 6.943 | 64.937 | 1.00 | 31.08 |
| ATOM | 3403 | O | LYS | B | 48 | 40.524 | 5.962 | 64.457 | 1.00 | 26.24 |
| ATOM | 3404 | N | SER | B | 49 | 41.260 | 7.121 | 66.244 | 1.00 | 27.89 |
| ATOM | 3405 | CA | SER | B | 49 | 40.770 | 6.168 | 67.232 | 1.00 | 25.17 |
| ATOM | 3406 | CB | SER | B | 49 | 41.146 | 6.639 | 68.642 | 1.00 | 24.41 |
| ATOM | 3407 | OG | SER | B | 49 | 42.539 | 6.858 | 68.777 | 1.00 | 31.79 |
| ATOM | 3408 | C | SER | B | 49 | 39.248 | 6.054 | 67.160 | 1.00 | 29.07 |
| ATOM | 3409 | O | SER | B | 49 | 38.565 | 7.034 | 66.879 | 1.00 | 28.47 |
| ATOM | 3410 | N | ARG | B | 50 | 38.723 | 4.859 | 67.409 | 1.00 | 26.13 |
| ATOM | 3411 | CA | ARG | B | 50 | 37.278 | 4.658 | 67.430 | 1.00 | 24.24 |
| ATOM | 3412 | CB | ARG | B | 50 | 36.810 | 3.700 | 66.323 | 1.00 | 25.03 |
| ATOM | 3413 | CG | ARG | B | 50 | 37.231 | 2.233 | 66.507 | 1.00 | 26.54 |
| ATOM | 3414 | CD | ARG | B | 50 | 36.570 | 1.340 | 65.452 | 1.00 | 26.21 |
| ATOM | 3415 | NE | ARG | B | 50 | 37.006 | -0.058 | 65.504 | 1.00 | 25.13 |
| ATOM | 3416 | CZ | ARG | B | 50 | 36.700 | -0.924 | 66.468 | 1.00 | 26.09 |
| ATOM | 3417 | NH1 | ARG | B | 50 | 35.941 | -0.558 | 67.497 | 1.00 | 23.42 |
| ATOM | 3418 | NH2 | ARG | B | 50 | 37.157 | -2.168 | 66.402 | 1.00 | 23.91 |
| ATOM | 3419 | C | ARG | B | 50 | 36.937 | 4.037 | 68.775 | 1.00 | 23.83 |
| ATOM | 3420 | O | ARG | B | 50 | 37.782 | 3.392 | 69.403 | 1.00 | 21.60 |
| ATOM | 3421 | N | PRO | B | 51 | 35.700 | 4.223 | 69.243 | 1.00 | 22.99 |
| ATOM | 3422 | CD | PRO | B | 51 | 34.554 | 4.962 | 68.688 | 1.00 | 25.09 |
| ATOM | 3423 | CA | PRO | B | 51 | 35.338 | 3.628 | 70.530 | 1.00 | 25.48 |
| ATOM | 3424 | CB | PRO | B | 51 | 33.949 | 4.217 | 70.802 | 1.00 | 26.32 |
| ATOM | 3425 | CG | PRO | B | 51 | 33.936 | 5.503 | 69.953 | 1.00 | 28.65 |
| ATOM | 3426 | C | PRO | B | 51 | 35.264 | 2.118 | 70.325 | 1.00 | 26.73 |
| ATOM | 3427 | O | PRO | B | 51 | 35.142 | 1.646 | 69.194 | 1.00 | 18.87 |
| ATOM | 3428 | N | ALA | B | 52 | 35.355 | 1.359 | 71.408 | 1.00 | 23.64 |
| ATOM | 3429 | CA | ALA | B | 52 | 35.237 | -0.083 | 71.291 | 1.00 | 23.27 |
| ATOM | 3430 | CB | ALA | B | 52 | 35.811 | -0.757 | 72.521 | 1.00 | 26.31 |
| ATOM | 3431 | C | ALA | B | 52 | 33.733 | -0.324 | 71.223 | 1.00 | 25.25 |
| ATOM | 3432 | O | ALA | B | 52 | 32.950 | 0.515 | 71.677 | 1.00 | 22.78 |
| ATOM | 3433 | N | THR | B | 53 | 33.321 | -1.447 | 70.651 | 1.00 | 22.77 |
| ATOM | 3434 | CA | THR | B | 53 | 31.900 | -1.760 | 70.596 | 1.00 | 26.90 |
| ATOM | 3435 | CB | THR | B | 53 | 31.567 | -2.732 | 69.456 | 1.00 | 30.00 |
| ATOM | 3436 | OG1 | THR | B | 53 | 32.305 | -3.950 | 69.642 | 1.00 | 25.59 |
| ATOM | 3437 | CG2 | THR | B | 53 | 31.917 | -2.117 | 68.103 | 1.00 | 23.33 |
| ATOM | 3438 | C | THR | B | 53 | 31.579 | -2.445 | 71.916 | 1.00 | 30.41 |
| ATOM | 3439 | O | THR | B | 53 | 32.484 | -2.917 | 72.609 | 1.00 | 26.13 |
| ATOM | 3440 | N | LYS | B | 54 | 30.300 | -2.504 | 72.268 | 1.00 | 29.12 |
| ATOM | 3441 | CA | LYS | B | 54 | 29.909 | -3.140 | 73.514 | 1.00 | 30.24 |
| ATOM | 3442 | CB | LYS | B | 54 | 28.396 | -3.027 | 73.720 | 1.00 | 32.78 |
| ATOM | 3443 | CG | LYS | B | 54 | 27.947 | -3.351 | 75.131 | 1.00 | 34.85 |
| ATOM | 3444 | CD | LYS | B | 54 | 26.445 | -3.204 | 75.268 | 1.00 | 41.13 |
| ATOM | 3445 | CE | LYS | B | 54 | 26.008 | -3.366 | 76.709 | 1.00 | 43.39 |
| ATOM | 3446 | NZ | LYS | B | 54 | 26.464 | -2.257 | 77.582 | 1.00 | 47.39 |
| ATOM | 3447 | C | LYS | B | 54 | 30.329 | -4.603 | 73.442 | 1.00 | 29.10 |
| ATOM | 3448 | O | LYS | B | 54 | 30.779 | -5.183 | 74.430 | 1.00 | 26.71 |
| ATOM | 3449 | N | GLU | B | 55 | 30.196 | -5.187 | 72.256 | 1.00 | 23.97 |
| ATOM | 3450 | CA | GLU | B | 55 | 30.577 | -6.577 | 72.032 | 1.00 | 28.08 |
| ATOM | 3451 | CB | GLU | B | 55 | 30.288 | -6.965 | 70.579 | 1.00 | 24.82 |
| ATOM | 3452 | CG | GLU | B | 55 | 30.671 | -8.400 | 70.237 | 1.00 | 33.40 |
| ATOM | 3453 | CD | GLU | B | 55 | 30.453 | -8.737 | 68.767 | 1.00 | 38.49 |
| ATOM | 3454 | OE1 | GLU | B | 55 | 30.638 | -9.913 | 68.394 | 1.00 | 41.24 |
| ATOM | 3455 | OE2 | GLU | B | 55 | 30.101 | -7.833 | 67.984 | 1.00 | 40.02 |

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Figure 18-53

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|---------|--------|------|-------|
| ATOM | 3456 | C | GLU | B | 55 | 32.066 | -6.808 | 72.345 | 1.00 | 25.82 |
| ATOM | 3457 | O | GLU | B | 55 | 32.429 | -7.765 | 73.033 | 1.00 | 23.83 |
| ATOM | 3458 | N | GLU | B | 56 | 32.931 | -5.938 | 71.835 | 1.00 | 25.04 |
| ATOM | 3459 | CA | GLU | B | 56 | 34.365 | -6.079 | 72.093 | 1.00 | 25.30 |
| ATOM | 3460 | CB | GLU | B | 56 | 35.141 | -5.003 | 71.334 | 1.00 | 24.31 |
| ATOM | 3461 | CG | GLU | B | 56 | 34.866 | -5.039 | 69.836 | 1.00 | 32.15 |
| ATOM | 3462 | CD | GLU | B | 56 | 35.512 | -3.903 | 69.073 | 1.00 | 31.43 |
| ATOM | 3463 | OE1 | GLU | B | 56 | 35.486 | -2.759 | 69.568 | 1.00 | 28.54 |
| ATOM | 3464 | OE2 | GLU | B | 56 | 36.012 | -4.147 | 67.959 | 1.00 | 28.89 |
| ATOM | 3465 | C | GLU | B | 56 | 34.653 | -5.988 | 73.595 | 1.00 | 28.88 |
| ATOM | 3466 | O | GLU | B | 56 | 35.450 | -6.766 | 74.137 | 1.00 | 25.07 |
| ATOM | 3467 | N | LEU | B | 57 | 33.996 | -5.050 | 74.272 | 1.00 | 24.52 |
| ATOM | 3468 | CA | LEU | B | 57 | 34.203 | -4.891 | 75.702 | 1.00 | 27.34 |
| ATOM | 3469 | CB | LEU | B | 57 | 33.416 | -3.694 | 76.231 | 1.00 | 22.79 |
| ATOM | 3470 | CG | LEU | B | 57 | 33.859 | -2.320 | 75.722 | 1.00 | 23.57 |
| ATOM | 3471 | CD1 | LEU | B | 57 | 33.008 | -1.247 | 76.366 | 1.00 | 22.27 |
| ATOM | 3472 | CD2 | LEU | B | 57 | 35.342 | -2.089 | 76.061 | 1.00 | 17.24 |
| ATOM | 3473 | C | LEU | B | 57 | 33.785 | -6.144 | 76.452 | 1.00 | 26.92 |
| ATOM | 3474 | O | LEU | B | 57 | 34.458 | -6.568 | 77.396 | 1.00 | 24.06 |
| ATOM | 3475 | N | LEU | B | 58 | 32.670 | -6.732 | 76.029 | 1.00 | 23.35 |
| ATOM | 3476 | CA | LEU | B | 58 | 32.154 | -7.931 | 76.674 | 1.00 | 25.60 |
| ATOM | 3477 | CB | LEU | B | 58 | 30.718 | -8.207 | 76.221 | 1.00 | 28.50 |
| ATOM | 3478 | CG | LEU | B | 58 | 29.734 | -7.110 | 76.649 | 1.00 | 30.91 |
| ATOM | 3479 | CD1 | LEU | B | 58 | 28.323 | -7.468 | 76.212 | 1.00 | 28.93 |
| ATOM | 3480 | CD2 | LEU | B | 58 | 29.794 | -6.945 | 78.157 | 1.00 | 33.44 |
| ATOM | 3481 | C | LEU | B | 58 | 33.027 | -9.153 | 76.446 | 1.00 | 24.59 |
| ATOM | 3482 | O | LEU | B | 58 | 32.760 | -10.216 | 76.991 | 1.00 | 19.76 |
| ATOM | 3483 | N | LEU | B | 59 | 34.065 | -9.006 | 75.630 | 1.00 | 23.99 |
| ATOM | 3484 | CA | LEU | B | 59 | 34.988 | -10.108 | 75.411 | 1.00 | 25.11 |
| ATOM | 3485 | CB | LEU | B | 59 | 36.018 | -9.757 | 74.332 | 1.00 | 21.64 |
| ATOM | 3486 | CG | LEU | B | 59 | 35.483 | -9.652 | 72.905 | 1.00 | 24.24 |
| ATOM | 3487 | CD1 | LEU | B | 59 | 36.585 | -9.177 | 71.975 | 1.00 | 24.25 |
| ATOM | 3488 | CD2 | LEU | B | 59 | 34.957 | -11.014 | 72.468 | 1.00 | 19.91 |
| ATOM | 3489 | C | LEU | B | 59 | 35.699 | -10.371 | 76.733 | 1.00 | 23.84 |
| ATOM | 3490 | O | LEU | B | 59 | 36.150 | -11.489 | 76.992 | 1.00 | 19.39 |
| ATOM | 3491 | N | PHE | B | 60 | 35.793 | -9.344 | 77.577 | 1.00 | 21.80 |
| ATOM | 3492 | CA | PHE | B | 60 | 36.462 | -9.510 | 78.876 | 1.00 | 23.08 |
| ATOM | 3493 | CB | PHE | B | 60 | 37.809 | -8.770 | 78.908 | 1.00 | 18.22 |
| ATOM | 3494 | CG | PHE | B | 60 | 38.544 | -8.906 | 80.230 | 1.00 | 21.72 |
| ATOM | 3495 | CD1 | PHE | B | 60 | 38.975 | -10.157 | 80.680 | 1.00 | 19.23 |
| ATOM | 3496 | CD2 | PHE | B | 60 | 38.757 | -7.791 | 81.048 | 1.00 | 17.75 |
| ATOM | 3497 | CE1 | PHE | B | 60 | 39.602 | -10.301 | 81.927 | 1.00 | 18.80 |
| ATOM | 3498 | CE2 | PHE | B | 60 | 39.384 | -7.923 | 82.297 | 1.00 | 19.23 |
| ATOM | 3499 | CZ | PHE | B | 60 | 39.807 | -9.184 | 82.737 | 1.00 | 16.10 |
| ATOM | 3500 | C | PHE | B | 60 | 35.648 | -9.069 | 80.083 | 1.00 | 21.58 |
| ATOM | 3501 | O | PHE | B | 60 | 35.508 | -9.822 | 81.040 | 1.00 | 22.21 |
| ATOM | 3502 | N | HIS | B | 61 | 35.128 | -7.847 | 80.055 | 1.00 | 20.65 |
| ATOM | 3503 | CA | HIS | B | 61 | 34.362 | -7.336 | 81.184 | 1.00 | 23.32 |
| ATOM | 3504 | CB | HIS | B | 61 | 34.422 | -5.807 | 81.229 | 1.00 | 27.60 |
| ATOM | 3505 | CG | HIS | B | 61 | 35.800 | -5.259 | 81.440 | 1.00 | 31.83 |
| ATOM | 3506 | CD2 | HIS | B | 61 | 36.466 | -4.940 | 82.575 | 1.00 | 26.86 |
| ATOM | 3507 | ND1 | HIS | B | 61 | 36.669 | -5.003 | 80.401 | 1.00 | 34.35 |
| ATOM | 3508 | CE1 | HIS | B | 61 | 37.810 | -4.546 | 80.887 | 1.00 | 34.78 |
| ATOM | 3509 | NE2 | HIS | B | 61 | 37.713 | -4.499 | 82.204 | 1.00 | 36.27 |
| ATOM | 3510 | C | HIS | B | 61 | 32.902 | -7.775 | 81.198 | 1.00 | 28.04 |
| ATOM | 3511 | O | HIS | B | 61 | 32.349 | -8.167 | 80.176 | 1.00 | 25.70 |
| ATOM | 3512 | N | THR | B | 62 | 32.276 | -7.691 | 82.367 | 1.00 | 25.25 |
| ATOM | 3513 | CA | THR | B | 62 | 30.882 | -8.084 | 82.506 | 1.00 | 25.35 |
| ATOM | 3514 | CB | THR | B | 62 | 30.578 | -8.549 | 83.932 | 1.00 | 25.47 |
| ATOM | 3515 | OG1 | THR | B | 62 | 30.783 | -7.462 | 84.843 | 1.00 | 28.62 |
| ATOM | 3516 | CG2 | THR | B | 62 | 31.482 | -9.701 | 84.315 | 1.00 | 21.32 |
| ATOM | 3517 | C | THR | B | 62 | 29.931 | -6.942 | 82.162 | 1.00 | 26.06 |
| ATOM | 3518 | O | THR | B | 62 | 30.287 | -5.771 | 82.254 | 1.00 | 24.14 |
| ATOM | 3519 | N | GLU | B | 63 | 28.718 | -7.305 | 81.759 | 1.00 | 28.01 |
| ATOM | 3520 | CA | GLU | B | 63 | 27.681 | -6.349 | 81.389 | 1.00 | 30.77 |
| ATOM | 3521 | CB | GLU | B | 63 | 26.374 | -7.094 | 81.114 | 1.00 | 33.97 |

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Figure 18-54

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3522 | CG | GLU | B | 63 | 25.213 | -6.210 | 80.667 | 1.00 | 41.12 |
| ATOM | 3523 | CD | GLU | B | 63 | 25.189 | -5.987 | 79.168 | 1.00 | 44.47 |
| ATOM | 3524 | OE1 | GLU | B | 63 | 24.361 | -5.177 | 78.689 | 1.00 | 42.64 |
| ATOM | 3525 | OE2 | GLU | B | 63 | 25.992 | -6.640 | 78.465 | 1.00 | 45.96 |
| ATOM | 3526 | C | GLU | B | 63 | 27.436 | -5.326 | 82.498 | 1.00 | 27.29 |
| ATOM | 3527 | O | GLU | B | 63 | 27.381 | -4.118 | 82.252 | 1.00 | 25.13 |
| ATOM | 3528 | N | ASP | B | 64 | 27.272 | -5.834 | 83.713 | 1.00 | 24.38 |
| ATOM | 3529 | CA | ASP | B | 64 | 27.010 | -5.023 | 84.897 | 1.00 | 29.27 |
| ATOM | 3530 | CB | ASP | B | 64 | 26.887 | -5.944 | 86.112 | 1.00 | 36.30 |
| ATOM | 3531 | CG | ASP | B | 64 | 28.022 | -6.935 | 86.198 | 1.00 | 50.77 |
| ATOM | 3532 | OD1 | ASP | B | 64 | 29.128 | -6.540 | 86.630 | 1.00 | 52.71 |
| ATOM | 3533 | OD2 | ASP | B | 64 | 27.812 | -8.106 | 85.802 | 1.00 | 51.98 |
| ATOM | 3534 | C | ASP | B | 64 | 28.075 | -3.967 | 85.143 | 1.00 | 26.49 |
| ATOM | 3535 | O | ASP | B | 64 | 27.768 | -2.806 | 85.422 | 1.00 | 18.33 |
| ATOM | 3536 | N | TYR | B | 65 | 29.332 | -4.373 | 85.052 | 1.00 | 22.75 |
| ATOM | 3537 | CA | TYR | B | 65 | 30.420 | -3.435 | 85.251 | 1.00 | 19.32 |
| ATOM | 3538 | CB | TYR | B | 65 | 31.751 | -4.186 | 85.256 | 1.00 | 16.59 |
| ATOM | 3539 | CG | TYR | B | 65 | 32.949 | -3.285 | 85.366 | 1.00 | 19.19 |
| ATOM | 3540 | CD1 | TYR | B | 65 | 33.033 | -2.328 | 86.383 | 1.00 | 21.35 |
| ATOM | 3541 | CE1 | TYR | B | 65 | 34.135 | -1.489 | 86.489 | 1.00 | 18.32 |
| ATOM | 3542 | CD2 | TYR | B | 65 | 34.004 | -3.382 | 84.456 | 1.00 | 18.65 |
| ATOM | 3543 | CE2 | TYR | B | 65 | 35.116 | -2.544 | 84.554 | 1.00 | 21.01 |
| ATOM | 3544 | CZ | TYR | B | 65 | 35.172 | -1.601 | 85.573 | 1.00 | 20.61 |
| ATOM | 3545 | OH | TYR | B | 65 | 36.262 | -0.775 | 85.682 | 1.00 | 17.77 |
| ATOM | 3546 | C | TYR | B | 65 | 30.392 | -2.373 | 84.146 | 1.00 | 22.01 |
| ATOM | 3547 | O | TYR | B | 65 | 30.399 | -1.167 | 84.421 | 1.00 | 18.20 |
| ATOM | 3548 | N | ILE | B | 66 | 30.330 | -2.815 | 82.894 | 1.00 | 19.49 |
| ATOM | 3549 | CA | ILE | B | 66 | 30.305 | -1.870 | 81.786 | 1.00 | 19.68 |
| ATOM | 3550 | CB | ILE | B | 66 | 30.208 | -2.592 | 80.432 | 1.00 | 23.31 |
| ATOM | 3551 | CG2 | ILE | B | 66 | 30.200 | -1.571 | 79.303 | 1.00 | 21.30 |
| ATOM | 3552 | CG1 | ILE | B | 66 | 31.400 | -3.541 | 80.260 | 1.00 | 27.67 |
| ATOM | 3553 | CD1 | ILE | B | 66 | 32.758 | -2.839 | 80.291 | 1.00 | 29.29 |
| ATOM | 3554 | C | ILE | B | 66 | 29.128 | -0.909 | 81.940 | 1.00 | 26.99 |
| ATOM | 3555 | O | ILE | B | 66 | 29.294 | 0.309 | 81.848 | 1.00 | 23.36 |
| ATOM | 3556 | N | ASN | B | 67 | 27.939 | -1.447 | 82.198 | 1.00 | 24.98 |
| ATOM | 3557 | CA | ASN | B | 67 | 26.782 | -0.580 | 82.363 | 1.00 | 27.70 |
| ATOM | 3558 | CB | ASN | B | 67 | 25.492 | -1.389 | 82.580 | 1.00 | 25.58 |
| ATOM | 3559 | CG | ASN | B | 67 | 25.081 | -2.183 | 81.341 | 1.00 | 26.91 |
| ATOM | 3560 | OD1 | ASN | B | 67 | 25.199 | -1.701 | 80.220 | 1.00 | 31.48 |
| ATOM | 3561 | ND2 | ASN | B | 67 | 24.572 | -3.387 | 81.545 | 1.00 | 23.80 |
| ATOM | 3562 | C | ASN | B | 67 | 26.982 | 0.401 | 83.513 | 1.00 | 25.34 |
| ATOM | 3563 | O | ASN | B | 67 | 26.524 | 1.539 | 83.448 | 1.00 | 22.53 |
| ATOM | 3564 | N | THR | B | 68 | 27.664 | -0.031 | 84.568 | 1.00 | 23.65 |
| ATOM | 3565 | CA | THR | B | 68 | 27.903 | 0.863 | 85.696 | 1.00 | 25.25 |
| ATOM | 3566 | CB | THR | B | 68 | 28.516 | 0.119 | 86.891 | 1.00 | 29.08 |
| ATOM | 3567 | OG1 | THR | B | 68 | 27.561 | -0.826 | 87.396 | 1.00 | 25.94 |
| ATOM | 3568 | CG2 | THR | B | 68 | 28.894 | 1.100 | 88.002 | 1.00 | 22.90 |
| ATOM | 3569 | C | THR | B | 68 | 28.818 | 2.009 | 85.287 | 1.00 | 25.91 |
| ATOM | 3570 | O | THR | B | 68 | 28.576 | 3.156 | 85.661 | 1.00 | 28.47 |
| ATOM | 3571 | N | LEU | B | 69 | 29.861 | 1.702 | 84.519 | 1.00 | 25.13 |
| ATOM | 3572 | CA | LEU | B | 69 | 30.788 | 2.729 | 84.054 | 1.00 | 24.37 |
| ATOM | 3573 | CB | LEU | B | 69 | 31.915 | 2.122 | 83.201 | 1.00 | 21.32 |
| ATOM | 3574 | CG | LEU | B | 69 | 32.960 | 1.231 | 83.889 | 1.00 | 22.33 |
| ATOM | 3575 | CD1 | LEU | B | 69 | 34.006 | 0.786 | 82.859 | 1.00 | 22.57 |
| ATOM | 3576 | CD2 | LEU | B | 69 | 33.643 | 2.000 | 85.008 | 1.00 | 23.20 |
| ATOM | 3577 | C | LEU | B | 69 | 30.036 | 3.764 | 83.229 | 1.00 | 23.02 |
| ATOM | 3578 | O | LEU | B | 69 | 30.190 | 4.966 | 83.444 | 1.00 | 18.98 |
| ATOM | 3579 | N | MET | B | 70 | 29.218 | 3.290 | 82.294 | 1.00 | 19.62 |
| ATOM | 3580 | CA | MET | B | 70 | 28.449 | 4.181 | 81.434 | 1.00 | 25.87 |
| ATOM | 3581 | CB | MET | B | 70 | 27.660 | 3.371 | 80.401 | 1.00 | 24.80 |
| ATOM | 3582 | CG | MET | B | 70 | 28.531 | 2.511 | 79.490 | 1.00 | 30.37 |
| ATOM | 3583 | SD | MET | B | 70 | 27.592 | 1.599 | 78.227 | 1.00 | 30.35 |
| ATOM | 3584 | CE | MET | B | 70 | 26.922 | 2.986 | 77.245 | 1.00 | 30.20 |
| ATOM | 3585 | C | MET | B | 70 | 27.489 | 5.062 | 82.242 | 1.00 | 28.82 |
| ATOM | 3586 | O | MET | B | 70 | 27.391 | 6.273 | 82.009 | 1.00 | 24.09 |
| ATOM | 3587 | N | GLU | B | 71 | 26.786 | 4.458 | 83.194 | 1.00 | 28.21 |

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Figure 18-55

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3588 | CA | GLU | B | 71 | 25.837 | 5.207 | 84.008 | 1.00 | 27.45 |
| ATOM | 3589 | CB | GLU | B | 71 | 25.014 | 4.268 | 84.889 | 1.00 | 30.70 |
| ATOM | 3590 | CG | GLU | B | 71 | 24.072 | 5.005 | 85.832 | 1.00 | 33.61 |
| ATOM | 3591 | CD | GLU | B | 71 | 23.044 | 5.867 | 85.096 | 1.00 | 37.51 |
| ATOM | 3592 | OE1 | GLU | B | 71 | 22.333 | 6.638 | 85.773 | 1.00 | 35.47 |
| ATOM | 3593 | OE2 | GLU | B | 71 | 22.934 | 5.769 | 83.849 | 1.00 | 31.03 |
| ATOM | 3594 | C | GLU | B | 71 | 26.559 | 6.209 | 84.887 | 1.00 | 29.15 |
| ATOM | 3595 | O | GLU | B | 71 | 26.115 | 7.341 | 85.035 | 1.00 | 23.96 |
| ATOM | 3596 | N | ALA | B | 72 | 27.671 | 5.781 | 85.481 | 1.00 | 27.76 |
| ATOM | 3597 | CA | ALA | B | 72 | 28.454 | 6.662 | 86.340 | 1.00 | 27.58 |
| ATOM | 3598 | CB | ALA | B | 72 | 29.663 | 5.920 | 86.909 | 1.00 | 23.24 |
| ATOM | 3599 | C | ALA | B | 72 | 28.924 | 7.886 | 85.563 | 1.00 | 28.07 |
| ATOM | 3600 | O | ALA | B | 72 | 28.895 | 8.999 | 86.079 | 1.00 | 23.22 |
| ATOM | 3601 | N | GLU | B | 73 | 29.356 | 7.684 | 84.322 | 1.00 | 26.40 |
| ATOM | 3602 | CA | GLU | B | 73 | 29.846 | 8.801 | 83.529 | 1.00 | 29.06 |
| ATOM | 3603 | CB | GLU | B | 73 | 30.658 | 8.314 | 82.325 | 1.00 | 29.48 |
| ATOM | 3604 | CG | GLU | B | 73 | 31.162 | 9.466 | 81.443 | 1.00 | 31.00 |
| ATOM | 3605 | CD | GLU | B | 73 | 31.938 | 9.009 | 80.216 | 1.00 | 34.37 |
| ATOM | 3606 | OE1 | GLU | B | 73 | 33.059 | 8.461 | 80.356 | 1.00 | 28.41 |
| ATOM | 3607 | OE2 | GLU | B | 73 | 31.419 | 9.203 | 79.100 | 1.00 | 30.59 |
| ATOM | 3608 | C | GLU | B | 73 | 28.744 | 9.734 | 83.045 | 1.00 | 31.92 |
| ATOM | 3609 | O | GLU | B | 73 | 28.894 | 10.951 | 83.104 | 1.00 | 35.69 |
| ATOM | 3610 | N | ARG | B | 74 | 27.633 | 9.186 | 82.570 | 1.00 | 33.53 |
| ATOM | 3611 | CA | ARG | B | 74 | 26.583 | 10.067 | 82.081 | 1.00 | 38.64 |
| ATOM | 3612 | CB | ARG | B | 74 | 25.456 | 9.280 | 81.403 | 1.00 | 39.90 |
| ATOM | 3613 | CG | ARG | B | 74 | 24.448 | 8.706 | 82.363 | 1.00 | 46.67 |
| ATOM | 3614 | CD | ARG | B | 74 | 23.174 | 8.311 | 81.646 | 1.00 | 47.53 |
| ATOM | 3615 | NE | ARG | B | 74 | 22.076 | 8.153 | 82.594 | 1.00 | 55.58 |
| ATOM | 3616 | CZ | ARG | B | 74 | 21.609 | 9.136 | 83.362 | 1.00 | 56.04 |
| ATOM | 3617 | NH1 | ARG | B | 74 | 22.142 | 10.351 | 83.297 | 1.00 | 58.93 |
| ATOM | 3618 | NH2 | ARG | B | 74 | 20.601 | 8.910 | 84.192 | 1.00 | 53.62 |
| ATOM | 3619 | C | ARG | B | 74 | 26.008 | 10.914 | 83.222 | 1.00 | 35.84 |
| ATOM | 3620 | O | ARG | B | 74 | 25.778 | 12.107 | 83.048 | 1.00 | 29.44 |
| ATOM | 3621 | N | SER | B | 75 | 25.794 | 10.302 | 84.386 | 1.00 | 31.02 |
| ATOM | 3622 | CA | SER | B | 75 | 25.243 | 11.014 | 85.539 | 1.00 | 31.99 |
| ATOM | 3623 | CB | SER | B | 75 | 24.592 | 10.038 | 86.510 | 1.00 | 34.47 |
| ATOM | 3624 | OG | SER | B | 75 | 25.581 | 9.228 | 87.123 | 1.00 | 34.33 |
| ATOM | 3625 | C | SER | B | 75 | 26.339 | 11.754 | 86.288 | 1.00 | 35.42 |
| ATOM | 3626 | O | SER | B | 75 | 26.060 | 12.555 | 87.180 | 1.00 | 33.45 |
| ATOM | 3627 | N | GLN | B | 76 | 27.584 | 11.473 | 85.922 | 1.00 | 33.25 |
| ATOM | 3628 | CA | GLN | B | 76 | 28.739 | 12.082 | 86.565 | 1.00 | 35.61 |
| ATOM | 3629 | CB | GLN | B | 76 | 28.818 | 13.572 | 86.241 | 1.00 | 30.11 |
| ATOM | 3630 | CG | GLN | B | 76 | 30.216 | 14.112 | 86.390 | 1.00 | 39.13 |
| ATOM | 3631 | CD | GLN | B | 76 | 31.124 | 13.681 | 85.248 | 1.00 | 33.54 |
| ATOM | 3632 | OE1 | GLN | B | 76 | 31.052 | 12.546 | 84.761 | 1.00 | 29.21 |
| ATOM | 3633 | NE2 | GLN | B | 76 | 31.995 | 14.583 | 84.827 | 1.00 | 40.93 |
| ATOM | 3634 | C | GLN | B | 76 | 28.624 | 11.892 | 88.079 | 1.00 | 37.88 |
| ATOM | 3635 | O | GLN | B | 76 | 28.901 | 12.908 | 88.858 | 1.00 | 32.74 |
| ATOM | 3636 | N | SER | B | 77 | 28.209 | 10.697 | 88.488 | 1.00 | 34.72 |
| ATOM | 3637 | CA | SER | B | 77 | 28.047 | 10.382 | 89.901 | 1.00 | 37.07 |
| ATOM | 3638 | CB | SER | B | 77 | 26.635 | 10.738 | 90.371 | 1.00 | 39.61 |
| ATOM | 3639 | OG | SER | B | 77 | 25.678 | 9.941 | 89.688 | 1.00 | 39.03 |
| ATOM | 3640 | C | SER | B | 77 | 28.265 | 8.897 | 90.112 | 1.00 | 35.95 |
| ATOM | 3641 | O | SER | B | 77 | 28.177 | 8.108 | 89.173 | 1.00 | 36.60 |
| ATOM | 3642 | N | VAL | B | 78 | 28.528 | 8.518 | 91.355 | 1.00 | 33.03 |
| ATOM | 3643 | CA | VAL | B | 78 | 28.753 | 7.124 | 91.685 | 1.00 | 33.41 |
| ATOM | 3644 | CB | VAL | B | 78 | 29.742 | 6.979 | 92.848 | 1.00 | 36.91 |
| ATOM | 3645 | CG1 | VAL | B | 78 | 29.955 | 5.499 | 93.163 | 1.00 | 34.37 |
| ATOM | 3646 | CG2 | VAL | B | 78 | 31.055 | 7.658 | 92.496 | 1.00 | 34.19 |
| ATOM | 3647 | C | VAL | B | 78 | 27.461 | 6.431 | 92.082 | 1.00 | 34.93 |
| ATOM | 3648 | O | VAL | B | 78 | 26.897 | 6.703 | 93.143 | 1.00 | 28.25 |
| ATOM | 3649 | N | PRO | B | 79 | 26.971 | 5.521 | 91.228 | 1.00 | 36.73 |
| ATOM | 3650 | CD | PRO | B | 79 | 27.532 | 5.114 | 89.930 | 1.00 | 37.44 |
| ATOM | 3651 | CA | PRO | B | 79 | 25.738 | 4.779 | 91.493 | 1.00 | 38.33 |
| ATOM | 3652 | CB | PRO | B | 79 | 25.668 | 3.826 | 90.301 | 1.00 | 38.68 |
| ATOM | 3653 | CG | PRO | B | 79 | 26.293 | 4.664 | 89.201 | 1.00 | 37.41 |

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Figure 18-56

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3654 | C | PRO | B | 79 | 25.788 | 4.046 | 92.834 | 1.00 | 36.92 |
| ATOM | 3655 | O | PRO | B | 79 | 26.854 | 3.648 | 93.298 | 1.00 | 33.03 |
| ATOM | 3656 | N | LYS | B | 80 | 24.623 | 3.881 | 93.448 | 1.00 | 38.43 |
| ATOM | 3657 | CA | LYS | B | 80 | 24.482 | 3.206 | 94.736 | 1.00 | 39.73 |
| ATOM | 3658 | CB | LYS | B | 80 | 23.003 | 2.871 | 94.967 | 1.00 | 43.33 |
| ATOM | 3659 | CG | LYS | B | 80 | 22.679 | 2.129 | 96.262 | 1.00 | 44.60 |
| ATOM | 3660 | CD | LYS | B | 80 | 21.198 | 1.742 | 96.287 | 1.00 | 48.09 |
| ATOM | 3661 | CE | LYS | B | 80 | 20.805 | 1.014 | 97.559 | 1.00 | 50.12 |
| ATOM | 3662 | NZ | LYS | B | 80 | 20.932 | 1.890 | 98.760 | 1.00 | 53.16 |
| ATOM | 3663 | C | LYS | B | 80 | 25.315 | 1.928 | 94.854 | 1.00 | 40.35 |
| ATOM | 3664 | O | LYS | B | 80 | 25.181 | 1.011 | 94.047 | 1.00 | 36.67 |
| ATOM | 3665 | N | GLY | B | 81 | 26.173 | 1.880 | 95.869 | 1.00 | 38.26 |
| ATOM | 3666 | CA | GLY | B | 81 | 26.996 | 0.709 | 96.104 | 1.00 | 34.69 |
| ATOM | 3667 | C | GLY | B | 81 | 28.066 | 0.407 | 95.071 | 1.00 | 34.63 |
| ATOM | 3668 | O | GLY | B | 81 | 28.861 | -0.513 | 95.255 | 1.00 | 33.92 |
| ATOM | 3669 | N | ALA | B | 82 | 28.100 | 1.178 | 93.992 | 1.00 | 31.26 |
| ATOM | 3670 | CA | ALA | B | 82 | 29.082 | 0.963 | 92.936 | 1.00 | 34.88 |
| ATOM | 3671 | CB | ALA | B | 82 | 28.755 | 1.848 | 91.751 | 1.00 | 23.13 |
| ATOM | 3672 | C | ALA | B | 82 | 30.517 | 1.223 | 93.405 | 1.00 | 36.85 |
| ATOM | 3673 | O | ALA | B | 82 | 31.461 | 0.580 | 92.945 | 1.00 | 32.17 |
| ATOM | 3674 | N | ARG | B | 83 | 30.677 | 2.168 | 94.323 | 1.00 | 36.52 |
| ATOM | 3675 | CA | ARG | B | 83 | 31.994 | 2.522 | 94.830 | 1.00 | 38.75 |
| ATOM | 3676 | CB | ARG | B | 83 | 31.865 | 3.616 | 95.885 | 1.00 | 40.24 |
| ATOM | 3677 | CG | ARG | B | 83 | 33.187 | 4.180 | 96.330 | 1.00 | 49.12 |
| ATOM | 3678 | CD | ARG | B | 83 | 33.015 | 5.239 | 97.404 | 1.00 | 53.26 |
| ATOM | 3679 | NE | ARG | B | 83 | 34.240 | 6.010 | 97.624 | 1.00 | 59.30 |
| ATOM | 3680 | CZ | ARG | B | 83 | 35.437 | 5.486 | 97.883 | 1.00 | 61.56 |
| ATOM | 3681 | NH1 | ARG | B | 83 | 35.598 | 4.170 | 97.958 | 1.00 | 63.53 |
| ATOM | 3682 | NH2 | ARG | B | 83 | 36.479 | 6.285 | 98.073 | 1.00 | 62.02 |
| ATOM | 3683 | C | ARG | B | 83 | 32.719 | 1.326 | 95.426 | 1.00 | 37.75 |
| ATOM | 3684 | O | ARG | B | 83 | 33.893 | 1.094 | 95.146 | 1.00 | 37.18 |
| ATOM | 3685 | N | GLU | B | 84 | 32.011 | 0.564 | 96.249 | 1.00 | 35.29 |
| ATOM | 3686 | CA | GLU | B | 84 | 32.581 | -0.609 | 96.898 | 1.00 | 35.29 |
| ATOM | 3687 | CB | GLU | B | 84 | 31.876 | -0.855 | 98.236 | 1.00 | 40.14 |
| ATOM | 3688 | CG | GLU | B | 84 | 30.443 | -0.383 | 98.240 | 1.00 | 46.30 |
| ATOM | 3689 | CD | GLU | B | 84 | 30.356 | 1.132 | 98.293 | 1.00 | 48.30 |
| ATOM | 3690 | OE1 | GLU | B | 84 | 29.339 | 1.690 | 97.834 | 1.00 | 43.07 |
| ATOM | 3691 | OE2 | GLU | B | 84 | 31.306 | 1.762 | 98.814 | 1.00 | 50.07 |
| ATOM | 3692 | C | GLU | B | 84 | 32.527 | -1.880 | 96.055 | 1.00 | 32.90 |
| ATOM | 3693 | O | GLU | B | 84 | 33.371 | -2.765 | 96.193 | 1.00 | 28.68 |
| ATOM | 3694 | N | LYS | B | 85 | 31.533 | -1.984 | 95.187 | 1.00 | 27.12 |
| ATOM | 3695 | CA | LYS | B | 85 | 31.412 | -3.177 | 94.361 | 1.00 | 30.46 |
| ATOM | 3696 | CB | LYS | B | 85 | 29.950 | -3.401 | 93.967 | 1.00 | 30.01 |
| ATOM | 3697 | CG | LYS | B | 85 | 29.717 | -4.643 | 93.117 | 1.00 | 28.40 |
| ATOM | 3698 | CD | LYS | B | 85 | 28.234 | -4.807 | 92.775 | 1.00 | 32.87 |
| ATOM | 3699 | CE | LYS | B | 85 | 28.000 | -6.048 | 91.928 | 1.00 | 34.15 |
| ATOM | 3700 | NZ | LYS | B | 85 | 26.582 | -6.186 | 91.507 | 1.00 | 35.34 |
| ATOM | 3701 | C | LYS | B | 85 | 32.267 | -3.096 | 93.101 | 1.00 | 28.98 |
| ATOM | 3702 | O | LYS | B | 85 | 32.817 | -4.098 | 92.652 | 1.00 | 24.69 |
| ATOM | 3703 | N | TYR | B | 86 | 32.391 | -1.896 | 92.550 | 1.00 | 27.81 |
| ATOM | 3704 | CA | TYR | B | 86 | 33.141 | -1.692 | 91.319 | 1.00 | 27.56 |
| ATOM | 3705 | CB | TYR | B | 86 | 32.206 | -1.050 | 90.288 | 1.00 | 28.88 |
| ATOM | 3706 | CG | TYR | B | 86 | 31.008 | -1.927 | 89.951 | 1.00 | 31.29 |
| ATOM | 3707 | CD1 | TYR | B | 86 | 31.178 | -3.137 | 89.276 | 1.00 | 26.99 |
| ATOM | 3708 | CE1 | TYR | B | 86 | 30.095 | -3.955 | 88.965 | 1.00 | 26.97 |
| ATOM | 3709 | CD2 | TYR | B | 86 | 29.713 | -1.553 | 90.315 | 1.00 | 28.38 |
| ATOM | 3710 | CE2 | TYR | B | 86 | 28.611 | -2.370 | 90.008 | 1.00 | 24.19 |
| ATOM | 3711 | CZ | TYR | B | 86 | 28.815 | -3.569 | 89.331 | 1.00 | 28.46 |
| ATOM | 3712 | OH | TYR | B | 86 | 27.747 | -4.379 | 89.008 | 1.00 | 22.70 |
| ATOM | 3713 | C | TYR | B | 86 | 34.422 | -0.870 | 91.489 | 1.00 | 24.64 |
| ATOM | 3714 | O | TYR | B | 86 | 35.160 | -0.645 | 90.530 | 1.00 | 27.19 |
| ATOM | 3715 | N | ASN | B | 87 | 34.674 | -0.418 | 92.711 | 1.00 | 25.54 |
| ATOM | 3716 | CA | ASN | B | 87 | 35.881 | 0.341 | 93.032 | 1.00 | 29.30 |
| ATOM | 3717 | CB | ASN | B | 87 | 37.105 | -0.561 | 92.866 | 1.00 | 28.92 |
| ATOM | 3718 | CG | ASN | B | 87 | 38.343 | 0.019 | 93.506 | 1.00 | 34.72 |
| ATOM | 3719 | OD1 | ASN | B | 87 | 38.309 | 0.452 | 94.659 | 1.00 | 38.41 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-57

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3720 | ND2 | ASN | B | 87 | 39.449 | 0.012 | 92.775 | 1.00 | 35.86 |
| ATOM | 3721 | C | ASN | B | 87 | 36.070 | 1.622 | 92.223 | 1.00 | 29.72 |
| ATOM | 3722 | O | ASN | B | 87 | 37.194 | 1.998 | 91.876 | 1.00 | 24.01 |
| ATOM | 3723 | N | ILE | B | 88 | 34.956 | 2.282 | 91.932 | 1.00 | 29.43 |
| ATOM | 3724 | CA | ILE | B | 88 | 34.945 | 3.536 | 91.196 | 1.00 | 30.64 |
| ATOM | 3725 | CB | ILE | B | 88 | 33.959 | 3.464 | 90.027 | 1.00 | 37.12 |
| ATOM | 3726 | CG2 | ILE | B | 88 | 33.821 | 4.829 | 89.379 | 1.00 | 40.62 |
| ATOM | 3727 | CG1 | ILE | B | 88 | 34.421 | 2.433 | 89.008 | 1.00 | 35.43 |
| ATOM | 3728 | CD1 | ILE | B | 88 | 35.684 | 2.821 | 88.324 | 1.00 | 41.80 |
| ATOM | 3729 | C | ILE | B | 88 | 34.483 | 4.669 | 92.118 | 1.00 | 31.90 |
| ATOM | 3730 | O | ILE | B | 88 | 33.681 | 4.445 | 93.024 | 1.00 | 28.86 |
| ATOM | 3731 | N | GLY | B | 89 | 34.977 | 5.881 | 91.875 | 1.00 | 30.36 |
| ATOM | 3732 | CA | GLY | B | 89 | 34.574 | 7.022 | 92.686 | 1.00 | 29.54 |
| ATOM | 3733 | C | GLY | B | 89 | 35.601 | 7.524 | 93.685 | 1.00 | 31.49 |
| ATOM | 3734 | O | GLY | B | 89 | 35.497 | 8.652 | 94.177 | 1.00 | 37.26 |
| ATOM | 3735 | N | GLY | B | 90 | 36.583 | 6.687 | 94.005 | 1.00 | 30.97 |
| ATOM | 3736 | CA | GLY | B | 90 | 37.612 | 7.086 | 94.949 | 1.00 | 31.03 |
| ATOM | 3737 | C | GLY | B | 90 | 38.655 | 7.936 | 94.247 | 1.00 | 34.78 |
| ATOM | 3738 | O | GLY | B | 90 | 38.455 | 8.344 | 93.103 | 1.00 | 32.73 |
| ATOM | 3739 | N | TYR | B | 91 | 39.772 | 8.201 | 94.915 | 1.00 | 29.39 |
| ATOM | 3740 | CA | TYR | B | 91 | 40.820 | 9.023 | 94.322 | 1.00 | 28.15 |
| ATOM | 3741 | CB | TYR | B | 91 | 41.810 | 9.463 | 95.405 | 1.00 | 27.29 |
| ATOM | 3742 | CG | TYR | B | 91 | 42.609 | 8.330 | 96.007 | 1.00 | 26.60 |
| ATOM | 3743 | CD1 | TYR | B | 91 | 43.738 | 7.823 | 95.359 | 1.00 | 28.55 |
| ATOM | 3744 | CE1 | TYR | B | 91 | 44.456 | 6.762 | 95.896 | 1.00 | 28.75 |
| ATOM | 3745 | CD2 | TYR | B | 91 | 42.219 | 7.741 | 97.208 | 1.00 | 28.35 |
| ATOM | 3746 | CE2 | TYR | B | 91 | 42.927 | 6.680 | 97.751 | 1.00 | 27.58 |
| ATOM | 3747 | CZ | TYR | B | 91 | 44.043 | 6.196 | 97.094 | 1.00 | 30.12 |
| ATOM | 3748 | OH | TYR | B | 91 | 44.753 | 5.154 | 97.637 | 1.00 | 36.59 |
| ATOM | 3749 | C | TYR | B | 91 | 41.563 | 8.271 | 93.226 | 1.00 | 29.27 |
| ATOM | 3750 | O | TYR | B | 91 | 42.109 | 8.874 | 92.308 | 1.00 | 25.22 |
| ATOM | 3751 | N | GLU | B | 92 | 41.568 | 6.948 | 93.318 | 1.00 | 28.32 |
| ATOM | 3752 | CA | GLU | B | 92 | 42.286 | 6.124 | 92.350 | 1.00 | 27.06 |
| ATOM | 3753 | CB | GLU | B | 92 | 42.474 | 4.726 | 92.924 | 1.00 | 23.35 |
| ATOM | 3754 | CG | GLU | B | 92 | 43.502 | 3.884 | 92.221 | 1.00 | 29.80 |
| ATOM | 3755 | CD | GLU | B | 92 | 43.585 | 2.500 | 92.826 | 1.00 | 35.34 |
| ATOM | 3756 | OE1 | GLU | B | 92 | 42.742 | 1.645 | 92.477 | 1.00 | 32.15 |
| ATOM | 3757 | OE2 | GLU | B | 92 | 44.475 | 2.278 | 93.678 | 1.00 | 31.61 |
| ATOM | 3758 | C | GLU | B | 92 | 41.594 | 6.024 | 90.997 | 1.00 | 23.42 |
| ATOM | 3759 | O | GLU | B | 92 | 42.204 | 6.260 | 89.962 | 1.00 | 20.47 |
| ATOM | 3760 | N | ASN | B | 93 | 40.314 | 5.677 | 91.017 | 1.00 | 18.85 |
| ATOM | 3761 | CA | ASN | B | 93 | 39.534 | 5.509 | 89.795 | 1.00 | 21.96 |
| ATOM | 3762 | CB | ASN | B | 93 | 39.165 | 4.033 | 89.664 | 1.00 | 23.90 |
| ATOM | 3763 | CG | ASN | B | 93 | 40.351 | 3.120 | 89.943 | 1.00 | 24.78 |
| ATOM | 3764 | OD1 | ASN | B | 93 | 41.362 | 3.160 | 89.239 | 1.00 | 22.35 |
| ATOM | 3765 | ND2 | ASN | B | 93 | 40.240 | 2.311 | 90.987 | 1.00 | 13.35 |
| ATOM | 3766 | C | ASN | B | 93 | 38.285 | 6.362 | 89.944 | 1.00 | 25.16 |
| ATOM | 3767 | O | ASN | B | 93 | 37.183 | 5.843 | 90.121 | 1.00 | 20.91 |
| ATOM | 3768 | N | PRO | B | 94 | 38.449 | 7.693 | 89.887 | 1.00 | 26.37 |
| ATOM | 3769 | CD | PRO | B | 94 | 39.738 | 8.389 | 89.716 | 1.00 | 19.35 |
| ATOM | 3770 | CA | PRO | B | 94 | 37.373 | 8.676 | 90.024 | 1.00 | 24.59 |
| ATOM | 3771 | CB | PRO | B | 94 | 38.147 | 9.972 | 90.200 | 1.00 | 25.95 |
| ATOM | 3772 | CG | PRO | B | 94 | 39.297 | 9.740 | 89.223 | 1.00 | 22.60 |
| ATOM | 3773 | C | PRO | B | 94 | 36.384 | 8.777 | 88.873 | 1.00 | 28.74 |
| ATOM | 3774 | O | PRO | B | 94 | 36.562 | 8.176 | 87.808 | 1.00 | 25.77 |
| ATOM | 3775 | N | VAL | B | 95 | 35.332 | 9.553 | 89.112 | 1.00 | 27.14 |
| ATOM | 3776 | CA | VAL | B | 95 | 34.317 | 9.812 | 88.103 | 1.00 | 25.94 |
| ATOM | 3777 | CB | VAL | B | 95 | 33.035 | 10.393 | 88.742 | 1.00 | 23.75 |
| ATOM | 3778 | CG1 | VAL | B | 95 | 32.067 | 10.855 | 87.662 | 1.00 | 26.34 |
| ATOM | 3779 | CG2 | VAL | B | 95 | 32.376 | 9.346 | 89.622 | 1.00 | 27.59 |
| ATOM | 3780 | C | VAL | B | 95 | 34.912 | 10.861 | 87.175 | 1.00 | 25.69 |
| ATOM | 3781 | O | VAL | B | 95 | 35.564 | 11.793 | 87.641 | 1.00 | 25.25 |
| ATOM | 3782 | N | SER | B | 96 | 34.708 | 10.699 | 85.871 | 1.00 | 28.02 |
| ATOM | 3783 | CA | SER | B | 96 | 35.199 | 11.647 | 84.868 | 1.00 | 24.82 |
| ATOM | 3784 | CB | SER | B | 96 | 36.729 | 11.705 | 84.850 | 1.00 | 25.90 |
| ATOM | 3785 | OG | SER | B | 96 | 37.274 | 10.548 | 84.229 | 1.00 | 23.99 |

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Figure 18-58

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3786 | C | SER | B | 96 | 34.726 | 11.127 | 83.519 | 1.00 | 26.22 |
| ATOM | 3787 | O | SER | B | 96 | 33.943 | 10.174 | 83.462 | 1.00 | 23.57 |
| ATOM | 3788 | N | TYR | B | 97 | 35.195 | 11.744 | 82.438 | 1.00 | 22.83 |
| ATOM | 3789 | CA | TYR | B | 97 | 34.818 | 11.279 | 81.110 | 1.00 | 28.59 |
| ATOM | 3790 | CB | TYR | B | 97 | 34.536 | 12.452 | 80.165 | 1.00 | 31.45 |
| ATOM | 3791 | CG | TYR | B | 97 | 33.279 | 13.203 | 80.548 | 1.00 | 35.09 |
| ATOM | 3792 | CD1 | TYR | B | 97 | 33.316 | 14.239 | 81.480 | 1.00 | 32.87 |
| ATOM | 3793 | CE1 | TYR | B | 97 | 32.148 | 14.863 | 81.911 | 1.00 | 37.73 |
| ATOM | 3794 | CD2 | TYR | B | 97 | 32.036 | 12.812 | 80.049 | 1.00 | 34.85 |
| ATOM | 3795 | CE2 | TYR | B | 97 | 30.858 | 13.430 | 80.475 | 1.00 | 38.61 |
| ATOM | 3796 | CZ | TYR | B | 97 | 30.924 | 14.453 | 81.408 | 1.00 | 39.45 |
| ATOM | 3797 | OH | TYR | B | 97 | 29.768 | 15.047 | 81.852 | 1.00 | 35.36 |
| ATOM | 3798 | C | TYR | B | 97 | 35.883 | 10.354 | 80.534 | 1.00 | 28.93 |
| ATOM | 3799 | O | TYR | B | 97 | 35.859 | 9.992 | 79.358 | 1.00 | 28.26 |
| ATOM | 3800 | N | ALA | B | 98 | 36.822 | 9.968 | 81.385 | 1.00 | 29.09 |
| ATOM | 3801 | CA | ALA | B | 98 | 37.866 | 9.044 | 80.980 | 1.00 | 26.88 |
| ATOM | 3802 | CB | ALA | B | 98 | 39.167 | 9.369 | 81.692 | 1.00 | 27.99 |
| ATOM | 3803 | C | ALA | B | 98 | 37.395 | 7.657 | 81.382 | 1.00 | 22.53 |
| ATOM | 3804 | O | ALA | B | 98 | 37.721 | 6.675 | 80.722 | 1.00 | 21.98 |
| ATOM | 3805 | N | MET | B | 99 | 36.603 | 7.595 | 82.453 | 1.00 | 23.51 |
| ATOM | 3806 | CA | MET | B | 99 | 36.106 | 6.326 | 82.986 | 1.00 | 26.36 |
| ATOM | 3807 | CB | MET | B | 99 | 35.179 | 6.568 | 84.185 | 1.00 | 24.05 |
| ATOM | 3808 | CG | MET | B | 99 | 33.822 | 7.188 | 83.875 | 1.00 | 28.37 |
| ATOM | 3809 | SD | MET | B | 99 | 32.966 | 7.704 | 85.406 | 1.00 | 27.91 |
| ATOM | 3810 | CE | MET | B | 99 | 33.106 | 6.227 | 86.409 | 1.00 | 22.12 |
| ATOM | 3811 | C | MET | B | 99 | 35.430 | 5.435 | 81.953 | 1.00 | 25.76 |
| ATOM | 3812 | O | MET | B | 99 | 35.544 | 4.212 | 82.031 | 1.00 | 26.11 |
| ATOM | 3813 | N | PHE | B | 100 | 34.724 | 6.027 | 80.992 | 1.00 | 22.17 |
| ATOM | 3814 | CA | PHE | B | 100 | 34.107 | 5.222 | 79.940 | 1.00 | 22.35 |
| ATOM | 3815 | CB | PHE | B | 100 | 32.582 | 5.133 | 80.088 | 1.00 | 22.01 |
| ATOM | 3816 | CG | PHE | B | 100 | 31.947 | 4.254 | 79.038 | 1.00 | 24.22 |
| ATOM | 3817 | CD1 | PHE | B | 100 | 32.143 | 2.872 | 79.061 | 1.00 | 26.61 |
| ATOM | 3818 | CD2 | PHE | B | 100 | 31.280 | 4.813 | 77.953 | 1.00 | 21.22 |
| ATOM | 3819 | CE1 | PHE | B | 100 | 31.691 | 2.059 | 78.012 | 1.00 | 26.91 |
| ATOM | 3820 | CE2 | PHE | B | 100 | 30.825 | 4.010 | 76.894 | 1.00 | 24.80 |
| ATOM | 3821 | CZ | PHE | B | 100 | 31.033 | 2.632 | 76.924 | 1.00 | 24.85 |
| ATOM | 3822 | C | PHE | B | 100 | 34.425 | 5.695 | 78.514 | 1.00 | 24.86 |
| ATOM | 3823 | O | PHE | B | 100 | 34.922 | 4.920 | 77.694 | 1.00 | 21.40 |
| ATOM | 3824 | N | THR | B | 101 | 34.131 | 6.957 | 78.204 | 1.00 | 24.24 |
| ATOM | 3825 | CA | THR | B | 101 | 34.390 | 7.469 | 76.854 | 1.00 | 24.54 |
| ATOM | 3826 | CB | THR | B | 101 | 33.914 | 8.926 | 76.708 | 1.00 | 24.46 |
| ATOM | 3827 | OG1 | THR | B | 101 | 32.504 | 8.985 | 76.953 | 1.00 | 27.64 |
| ATOM | 3828 | CG2 | THR | B | 101 | 34.191 | 9.445 | 75.297 | 1.00 | 22.19 |
| ATOM | 3829 | C | THR | B | 101 | 35.872 | 7.387 | 76.483 | 1.00 | 25.26 |
| ATOM | 3830 | O | THR | B | 101 | 36.231 | 6.856 | 75.430 | 1.00 | 25.47 |
| ATOM | 3831 | N | GLY | B | 102 | 36.725 | 7.916 | 77.350 | 1.00 | 23.74 |
| ATOM | 3832 | CA | GLY | B | 102 | 38.153 | 7.867 | 77.096 | 1.00 | 24.53 |
| ATOM | 3833 | C | GLY | B | 102 | 38.657 | 6.434 | 77.046 | 1.00 | 24.06 |
| ATOM | 3834 | O | GLY | B | 102 | 39.346 | 6.045 | 76.100 | 1.00 | 22.53 |
| ATOM | 3835 | N | SER | B | 103 | 38.316 | 5.651 | 78.067 | 1.00 | 22.02 |
| ATOM | 3836 | CA | SER | B | 103 | 38.730 | 4.253 | 78.146 | 1.00 | 20.45 |
| ATOM | 3837 | CB | SER | B | 103 | 38.193 | 3.613 | 79.427 | 1.00 | 25.21 |
| ATOM | 3838 | OG | SER | B | 103 | 38.820 | 4.166 | 80.567 | 1.00 | 26.48 |
| ATOM | 3839 | C | SER | B | 103 | 38.268 | 3.446 | 76.938 | 1.00 | 20.53 |
| ATOM | 3840 | O | SER | B | 103 | 39.034 | 2.669 | 76.372 | 1.00 | 16.82 |
| ATOM | 3841 | N | SER | B | 104 | 37.014 | 3.642 | 76.542 | 1.00 | 17.11 |
| ATOM | 3842 | CA | SER | B | 104 | 36.462 | 2.937 | 75.395 | 1.00 | 23.32 |
| ATOM | 3843 | CB | SER | B | 104 | 34.980 | 3.289 | 75.228 | 1.00 | 22.93 |
| ATOM | 3844 | OG | SER | B | 104 | 34.424 | 2.557 | 74.161 | 1.00 | 24.75 |
| ATOM | 3845 | C | SER | B | 104 | 37.221 | 3.288 | 74.116 | 1.00 | 21.97 |
| ATOM | 3846 | O | SER | B | 104 | 37.451 | 2.434 | 73.256 | 1.00 | 22.83 |
| ATOM | 3847 | N | LEU | B | 105 | 37.619 | 4.549 | 73.997 | 1.00 | 23.00 |
| ATOM | 3848 | CA | LEU | B | 105 | 38.354 | 5.007 | 72.825 | 1.00 | 25.12 |
| ATOM | 3849 | CB | LEU | B | 105 | 38.443 | 6.536 | 72.859 | 1.00 | 29.25 |
| ATOM | 3850 | CG | LEU | B | 105 | 38.702 | 7.289 | 71.553 | 1.00 | 34.27 |
| ATOM | 3851 | CD1 | LEU | B | 105 | 37.662 | 6.888 | 70.512 | 1.00 | 31.51 |

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Figure 18-59

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3852 | CD2 | LEU | B | 105 | 38.629 | 8.802 | 71.819 | 1.00 | 34.30 |
| ATOM | 3853 | C | LEU | B | 105 | 39.755 | 4.374 | 72.813 | 1.00 | 27.39 |
| ATOM | 3854 | O | LEU | B | 105 | 40.262 | 3.955 | 71.765 | 1.00 | 20.15 |
| ATOM | 3855 | N | ALA | B | 106 | 40.371 | 4.293 | 73.988 | 1.00 | 23.62 |
| ATOM | 3856 | CA | ALA | B | 106 | 41.704 | 3.692 | 74.115 | 1.00 | 22.73 |
| ATOM | 3857 | CB | ALA | B | 106 | 42.263 | 3.939 | 75.529 | 1.00 | 17.46 |
| ATOM | 3858 | C | ALA | B | 106 | 41.639 | 2.189 | 73.846 | 1.00 | 22.77 |
| ATOM | 3859 | O | ALA | B | 106 | 42.583 | 1.597 | 73.316 | 1.00 | 24.98 |
| ATOM | 3860 | N | THR | B | 107 | 40.523 | 1.567 | 74.224 | 1.00 | 23.54 |
| ATOM | 3861 | CA | THR | B | 107 | 40.355 | 0.132 | 74.033 | 1.00 | 19.76 |
| ATOM | 3862 | CB | THR | B | 107 | 39.236 | -0.410 | 74.947 | 1.00 | 22.85 |
| ATOM | 3863 | OG1 | THR | B | 107 | 39.572 | -0.128 | 76.306 | 1.00 | 16.29 |
| ATOM | 3864 | CG2 | THR | B | 107 | 39.085 | -1.917 | 74.787 | 1.00 | 17.21 |
| ATOM | 3865 | C | THR | B | 107 | 40.036 | -0.169 | 72.571 | 1.00 | 23.47 |
| ATOM | 3866 | O | THR | B | 107 | 40.540 | -1.138 | 72.001 | 1.00 | 19.25 |
| ATOM | 3867 | N | GLY | B | 108 | 39.191 | 0.656 | 71.959 | 1.00 | 24.87 |
| ATOM | 3868 | CA | GLY | B | 108 | 38.879 | 0.434 | 70.560 | 1.00 | 21.32 |
| ATOM | 3869 | C | GLY | B | 108 | 40.161 | 0.594 | 69.757 | 1.00 | 22.01 |
| ATOM | 3870 | O | GLY | B | 108 | 40.388 | -0.099 | 68.761 | 1.00 | 20.46 |
| ATOM | 3871 | N | SER | B | 109 | 41.018 | 1.508 | 70.197 | 1.00 | 19.89 |
| ATOM | 3872 | CA | SER | B | 109 | 42.274 | 1.749 | 69.499 | 1.00 | 19.37 |
| ATOM | 3873 | CB | SER | B | 109 | 42.993 | 2.956 | 70.107 | 1.00 | 18.28 |
| ATOM | 3874 | OG | SER | B | 109 | 42.250 | 4.145 | 69.882 | 1.00 | 21.29 |
| ATOM | 3875 | C | SER | B | 109 | 43.168 | 0.513 | 69.542 | 1.00 | 20.70 |
| ATOM | 3876 | O | SER | B | 109 | 43.940 | 0.261 | 68.617 | 1.00 | 20.69 |
| ATOM | 3877 | N | THR | B | 110 | 43.065 | -0.259 | 70.616 | 1.00 | 20.54 |
| ATOM | 3878 | CA | THR | B | 110 | 43.858 | -1.475 | 70.729 | 1.00 | 19.98 |
| ATOM | 3879 | CB | THR | B | 110 | 43.826 | -2.043 | 72.158 | 1.00 | 20.63 |
| ATOM | 3880 | OG1 | THR | B | 110 | 44.632 | -1.215 | 73.007 | 1.00 | 20.72 |
| ATOM | 3881 | CG2 | THR | B | 110 | 44.371 | -3.470 | 72.188 | 1.00 | 20.05 |
| ATOM | 3882 | C | THR | B | 110 | 43.333 | -2.507 | 69.738 | 1.00 | 21.61 |
| ATOM | 3883 | O | THR | B | 110 | 44.115 | -3.239 | 69.127 | 1.00 | 18.11 |
| ATOM | 3884 | N | VAL | B | 111 | 42.012 | -2.557 | 69.567 | 1.00 | 18.29 |
| ATOM | 3885 | CA | VAL | B | 111 | 41.432 | -3.486 | 68.608 | 1.00 | 20.36 |
| ATOM | 3886 | CB | VAL | B | 111 | 39.886 | -3.494 | 68.677 | 1.00 | 23.94 |
| ATOM | 3887 | CG1 | VAL | B | 111 | 39.324 | -4.442 | 67.619 | 1.00 | 24.37 |
| ATOM | 3888 | CG2 | VAL | B | 111 | 39.426 | -3.937 | 70.063 | 1.00 | 21.60 |
| ATOM | 3889 | C | VAL | B | 111 | 41.872 | -3.080 | 67.197 | 1.00 | 20.35 |
| ATOM | 3890 | O | VAL | B | 111 | 42.146 | -3.936 | 66.362 | 1.00 | 23.29 |
| ATOM | 3891 | N | GLN | B | 112 | 41.953 | -1.775 | 66.937 | 1.00 | 22.07 |
| ATOM | 3892 | CA | GLN | B | 112 | 42.367 | -1.290 | 65.617 | 1.00 | 22.34 |
| ATOM | 3893 | CB | GLN | B | 112 | 42.199 | 0.230 | 65.513 | 1.00 | 24.54 |
| ATOM | 3894 | CG | GLN | B | 112 | 40.810 | 0.729 | 65.843 | 1.00 | 20.63 |
| ATOM | 3895 | CD | GLN | B | 112 | 40.700 | 2.236 | 65.742 | 1.00 | 21.19 |
| ATOM | 3896 | OE1 | GLN | B | 112 | 40.664 | 2.794 | 64.645 | 1.00 | 26.73 |
| ATOM | 3897 | NE2 | GLN | B | 112 | 40.667 | 2.905 | 66.886 | 1.00 | 18.73 |
| ATOM | 3898 | C | GLN | B | 112 | 43.826 | -1.635 | 65.363 | 1.00 | 23.1 |
| ATOM | 3899 | O | GLN | B | 112 | 44.195 | -2.020 | 64.257 | 1.00 | 15.79 |
| ATOM | 3900 | N | ALA | B | 113 | 44.660 | -1.476 | 66.389 | 1.00 | 20.60 |
| ATOM | 3901 | CA | ALA | B | 113 | 46.070 | -1.790 | 66.249 | 1.00 | 18.02 |
| ATOM | 3902 | CB | ALA | B | 113 | 46.794 | -1.536 | 67.548 | 1.00 | 20.84 |
| ATOM | 3903 | C | ALA | B | 113 | 46.170 | -3.262 | 65.863 | 1.00 | 23.78 |
| ATOM | 3904 | O | ALA | B | 113 | 46.982 | -3.642 | 65.023 | 1.00 | 19.83 |
| ATOM | 3905 | N | ILE | B | 114 | 45.331 | -4.091 | 66.477 | 1.00 | 21.45 |
| ATOM | 3906 | CA | ILE | B | 114 | 45.344 | -5.511 | 66.168 | 1.00 | 24.26 |
| ATOM | 3907 | CB | ILE | B | 114 | 44.507 | -6.306 | 67.191 | 1.00 | 20.72 |
| ATOM | 3908 | CG2 | ILE | B | 114 | 44.476 | -7.779 | 66.800 | 1.00 | 21.92 |
| ATOM | 3909 | CG1 | ILE | B | 114 | 45.116 | -6.144 | 68.593 | 1.00 | 24.32 |
| ATOM | 3910 | CD1 | ILE | B | 114 | 44.364 | -6.872 | 69.694 | 1.00 | 19.01 |
| ATOM | 3911 | C | ILE | B | 114 | 44.808 | -5.765 | 64.753 | 1.00 | 26.75 |
| ATOM | 3912 | O | ILE | B | 114 | 45.305 | -6.640 | 64.032 | 1.00 | 20.18 |
| ATOM | 3913 | N | GLU | B | 115 | 43.792 | -5.009 | 64.347 | 1.00 | 24.69 |
| ATOM | 3914 | CA | GLU | B | 115 | 43.243 | -5.198 | 63.005 | 1.00 | 29.26 |
| ATOM | 3915 | CB | GLU | B | 115 | 42.043 | -4.278 | 62.770 | 1.00 | 29.07 |
| ATOM | 3916 | CG | GLU | B | 115 | 40.940 | -4.421 | 63.800 | 1.00 | 32.31 |
| ATOM | 3917 | CD | GLU | B | 115 | 39.757 | -3.519 | 63.516 | 1.00 | 38.14 |

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Figure 18-60

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 3918 | OE1 | GLU | B | 115 | 39.980 | -2.374 | 63.072 | 1.00 | 40.63 |
| ATOM | 3919 | OE2 | GLU | B | 115 | 38.607 | -3.940 | 63.758 | 1.00 | 39.86 |
| ATOM | 3920 | C | GLU | B | 115 | 44.334 | -4.906 | 61.974 | 1.00 | 31.52 |
| ATOM | 3921 | O | GLU | B | 115 | 44.444 | -5.603 | 60.964 | 1.00 | 26.43 |
| ATOM | 3922 | N | GLU | B | 116 | 45.141 | -3.879 | 62.234 | 1.00 | 26.04 |
| ATOM | 3923 | CA | GLU | B | 116 | 46.226 | -3.522 | 61.324 | 1.00 | 26.21 |
| ATOM | 3924 | CB | GLU | B | 116 | 46.909 | -2.227 | 61.775 | 1.00 | 23.21 |
| ATOM | 3925 | CG | GLU | B | 116 | 46.055 | -0.983 | 61.601 | 1.00 | 23.82 |
| ATOM | 3926 | CD | GLU | B | 116 | 45.576 | -0.817 | 60.163 | 1.00 | 31.43 |
| ATOM | 3927 | OE1 | GLU | B | 116 | 46.425 | -0.734 | 59.253 | 1.00 | 26.45 |
| ATOM | 3928 | OE2 | GLU | B | 116 | 44.349 | -0.771 | 59.945 | 1.00 | 24.59 |
| ATOM | 3929 | C | GLU | B | 116 | 47.256 | -4.644 | 61.243 | 1.00 | 28.60 |
| ATOM | 3930 | O | GLU | B | 116 | 47.857 | -4.884 | 60.189 | 1.00 | 25.01 |
| ATOM | 3931 | N | PHE | B | 117 | 47.470 | -5.324 | 62.363 | 1.00 | 26.22 |
| ATOM | 3932 | CA | PHE | B | 117 | 48.421 | -6.425 | 62.400 | 1.00 | 28.05 |
| ATOM | 3933 | CB | PHE | B | 117 | 48.516 | -7.007 | 63.805 | 1.00 | 32.15 |
| ATOM | 3934 | CG | PHE | B | 117 | 49.278 | -8.299 | 63.869 | 1.00 | 33.88 |
| ATOM | 3935 | CD1 | PHE | B | 117 | 50.656 | -8.321 | 63.713 | 1.00 | 33.52 |
| ATOM | 3936 | CD2 | PHE | B | 117 | 48.604 | -9.502 | 64.054 | 1.00 | 32.83 |
| ATOM | 3937 | CE1 | PHE | B | 117 | 51.356 | -9.521 | 63.740 | 1.00 | 31.67 |
| ATOM | 3938 | CE2 | PHE | B | 117 | 49.294 | -10.710 | 64.082 | 1.00 | 35.69 |
| ATOM | 3939 | CZ | PHE | B | 117 | 50.674 | -10.717 | 63.926 | 1.00 | 36.72 |
| ATOM | 3940 | C | PHE | B | 117 | 47.929 | -7.508 | 61.456 | 1.00 | 26.43 |
| ATOM | 3941 | O | PHE | B | 117 | 48.689 | -8.061 | 60.669 | 1.00 | 27.61 |
| ATOM | 3942 | N | LEU | B | 118 | 46.642 | -7.809 | 61.551 | 1.00 | 23.59 |
| ATOM | 3943 | CA | LEU | B | 118 | 46.048 | -8.820 | 60.705 | 1.00 | 29.15 |
| ATOM | 3944 | CB | LEU | B | 118 | 44.585 | -9.039 | 61.099 | 1.00 | 28.78 |
| ATOM | 3945 | CG | LEU | B | 118 | 44.375 | -9.478 | 62.557 | 1.00 | 35.24 |
| ATOM | 3946 | CD1 | LEU | B | 118 | 42.898 | -9.763 | 62.788 | 1.00 | 31.92 |
| ATOM | 3947 | CD2 | LEU | B | 118 | 45.205 | -10.723 | 62.856 | 1.00 | 33.40 |
| ATOM | 3948 | C | LEU | B | 118 | 46.153 | -8.422 | 59.236 | 1.00 | 30.15 |
| ATOM | 3949 | O | LEU | B | 118 | 46.350 | -9.276 | 58.379 | 1.00 | 27.04 |
| ATOM | 3950 | N | LYS | B | 119 | 46.035 | -7.128 | 58.947 | 1.00 | 27.96 |
| ATOM | 3951 | CA | LYS | B | 119 | 46.127 | -6.663 | 57.569 | 1.00 | 26.69 |
| ATOM | 3952 | CB | LYS | B | 119 | 45.470 | -5.291 | 57.412 | 1.00 | 23.94 |
| ATOM | 3953 | CG | LYS | B | 119 | 43.998 | -5.260 | 57.795 | 1.00 | 24.41 |
| ATOM | 3954 | CD | LYS | B | 119 | 43.327 | -3.970 | 57.350 | 1.00 | 27.53 |
| ATOM | 3955 | CE | LYS | B | 119 | 44.024 | -2.739 | 57.886 | 1.00 | 33.13 |
| ATOM | 3956 | NZ | LYS | B | 119 | 43.371 | -1.479 | 57.428 | 1.00 | 27.75 |
| ATOM | 3957 | C | LYS | B | 119 | 47.577 | -6.598 | 57.101 | 1.00 | 29.12 |
| ATOM | 3958 | O | LYS | B | 119 | 47.864 | -6.160 | 55.984 | 1.00 | 35.25 |
| ATOM | 3959 | N | GLY | B | 120 | 48.493 | -7.034 | 57.958 | 1.00 | 30.25 |
| ATOM | 3960 | CA | GLY | B | 120 | 49.896 | -7.037 | 57.585 | 1.00 | 28.38 |
| ATOM | 3961 | C | GLY | B | 120 | 50.642 | -5.751 | 57.861 | 1.00 | 27.91 |
| ATOM | 3962 | O | GLY | B | 120 | 51.775 | -5.582 | 57.403 | 1.00 | 22.25 |
| ATOM | 3963 | N | ASN | B | 121 | 50.024 | -4.836 | 58.600 | 1.00 | 25.42 |
| ATOM | 3964 | CA | ASN | B | 121 | 50.695 | -3.587 | 58.919 | 1.00 | 29.49 |
| ATOM | 3965 | CB | ASN | B | 121 | 49.758 | -2.389 | 58.727 | 1.00 | 30.07 |
| ATOM | 3966 | CG | ASN | B | 121 | 49.201 | -2.307 | 57.325 | 1.00 | 32.25 |
| ATOM | 3967 | OD1 | ASN | B | 121 | 49.924 | -2.491 | 56.350 | 1.00 | 35.44 |
| ATOM | 3968 | ND2 | ASN | B | 121 | 47.917 | -2.006 | 57.217 | 1.00 | 32.26 |
| ATOM | 3969 | C | ASN | B | 121 | 51.172 | -3.637 | 60.361 | 1.00 | 30.92 |
| ATOM | 3970 | O | ASN | B | 121 | 50.971 | -4.631 | 61.059 | 1.00 | 27.08 |
| ATOM | 3971 | N | VAL | B | 122 | 51.810 | -2.560 | 60.796 | 1.00 | 28.46 |
| ATOM | 3972 | CA | VAL | B | 122 | 52.309 | -2.457 | 62.155 | 1.00 | 29.48 |
| ATOM | 3973 | CB | VAL | B | 122 | 53.840 | -2.352 | 62.177 | 1.00 | 33.40 |
| ATOM | 3974 | CG1 | VAL | B | 122 | 54.334 | -2.294 | 63.611 | 1.00 | 32.22 |
| ATOM | 3975 | CG2 | VAL | B | 122 | 54.446 | -3.544 | 61.458 | 1.00 | 33.57 |
| ATOM | 3976 | C | VAL | B | 122 | 51.713 | -1.196 | 62.748 | 1.00 | 29.04 |
| ATOM | 3977 | O | VAL | B | 122 | 51.800 | -0.118 | 62.153 | 1.00 | 27.47 |
| ATOM | 3978 | N | ALA | B | 123 | 51.100 | -1.326 | 63.918 | 1.00 | 26.71 |
| ATOM | 3979 | CA | ALA | B | 123 | 50.477 | -0.177 | 64.559 | 1.00 | 25.62 |
| ATOM | 3980 | CB | ALA | B | 123 | 48.963 | -0.281 | 64.447 | 1.00 | 21.65 |
| ATOM | 3981 | C | ALA | B | 123 | 50.872 | -0.005 | 66.017 | 1.00 | 28.62 |
| ATOM | 3982 | O | ALA | B | 123 | 51.227 | -0.965 | 66.712 | 1.00 | 26.96 |
| ATOM | 3983 | N | PHE | B | 124 | 50.805 | 1.239 | 66.472 | 1.00 | 22.85 |

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Figure 18-61

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3984 | CA | PHE | B | 124 | 51.122 | 1.577 | 67.847 | 1.00 | 17.31 |
| ATOM | 3985 | CB | PHE | B | 124 | 52.419 | 2.404 | 67.876 | 1.00 | 16.88 |
| ATOM | 3986 | CG | PHE | B | 124 | 52.762 | 3.000 | 69.225 | 1.00 | 18.52 |
| ATOM | 3987 | CD1 | PHE | B | 124 | 52.533 | 2.304 | 70.403 | 1.00 | 17.52 |
| ATOM | 3988 | CD2 | PHE | B | 124 | 53.382 | 4.245 | 69.297 | 1.00 | 17.88 |
| ATOM | 3989 | CE1 | PHE | B | 124 | 52.914 | 2.837 | 71.638 | 1.00 | 25.77 |
| ATOM | 3990 | CE2 | PHE | B | 124 | 53.769 | 4.790 | 70.517 | 1.00 | 21.97 |
| ATOM | 3991 | CZ | PHE | B | 124 | 53.535 | 4.084 | 71.698 | 1.00 | 20.16 |
| ATOM | 3992 | C | PHE | B | 124 | 49.937 | 2.348 | 68.421 | 1.00 | 18.77 |
| ATOM | 3993 | O | PHE | B | 124 | 49.462 | 3.311 | 67.820 | 1.00 | 16.62 |
| ATOM | 3994 | N | ASN | B | 125 | 49.418 | 1.868 | 69.546 | 1.00 | 16.69 |
| ATOM | 3995 | CA | ASN | B | 125 | 48.320 | 2.528 | 70.238 | 1.00 | 16.22 |
| ATOM | 3996 | CB | ASN | B | 125 | 47.129 | 1.603 | 70.435 | 1.00 | 12.71 |
| ATOM | 3997 | CG | ASN | B | 125 | 46.095 | 2.209 | 71.346 | 1.00 | 19.79 |
| ATOM | 3998 | OD1 | ASN | B | 125 | 45.930 | 3.430 | 71.372 | 1.00 | 20.83 |
| ATOM | 3999 | ND2 | ASN | B | 125 | 45.376 | 1.371 | 72.087 | 1.00 | 12.31 |
| ATOM | 4000 | C | ASN | B | 125 | 48.790 | 3.004 | 71.600 | 1.00 | 19.19 |
| ATOM | 4001 | O | ASN | B | 125 | 48.687 | 2.280 | 72.585 | 1.00 | 20.99 |
| ATOM | 4002 | N | PRO | B | 126 | 49.335 | 4.226 | 71.668 | 1.00 | 19.02 |
| ATOM | 4003 | CD | PRO | B | 126 | 49.595 | 5.156 | 70.555 | 1.00 | 21.39 |
| ATOM | 4004 | CA | PRO | B | 126 | 49.833 | 4.805 | 72.917 | 1.00 | 21.60 |
| ATOM | 4005 | CB | PRO | B | 126 | 50.398 | 6.161 | 72.459 | 1.00 | 21.07 |
| ATOM | 4006 | CG | PRO | B | 126 | 49.530 | 6.487 | 71.269 | 1.00 | 17.70 |
| ATOM | 4007 | C | PRO | B | 126 | 48.808 | 4.942 | 74.034 | 1.00 | 20.69 |
| ATOM | 4008 | O | PRO | B | 126 | 49.178 | 5.053 | 75.198 | 1.00 | 19.79 |
| ATOM | 4009 | N | ALA | B | 127 | 47.525 | 4.937 | 73.689 | 1.00 | 16.67 |
| ATOM | 4010 | CA | ALA | B | 127 | 46.476 | 5.065 | 74.698 | 1.00 | 20.44 |
| ATOM | 4011 | CB | ALA | B | 127 | 45.198 | 5.609 | 74.066 | 1.00 | 19.56 |
| ATOM | 4012 | C | ALA | B | 127 | 46.169 | 3.747 | 75.401 | 1.00 | 20.80 |
| ATOM | 4013 | O | ALA | B | 127 | 45.555 | 3.742 | 76.472 | 1.00 | 19.47 |
| ATOM | 4014 | N | GLY | B | 128 | 46.587 | 2.634 | 74.800 | 1.00 | 20.52 |
| ATOM | 4015 | CA | GLY | B | 128 | 46.325 | 1.333 | 75.399 | 1.00 | 19.43 |
| ATOM | 4016 | C | GLY | B | 128 | 47.327 | 0.910 | 76.463 | 1.00 | 20.56 |
| ATOM | 4017 | O | GLY | B | 128 | 48.182 | 1.697 | 76.869 | 1.00 | 18.37 |
| ATOM | 4018 | N | GLY | B | 129 | 47.215 | -0.333 | 76.929 | 1.00 | 19.68 |
| ATOM | 4019 | CA | GLY | B | 129 | 48.136 | -0.820 | 77.943 | 1.00 | 19.93 |
| ATOM | 4020 | C | GLY | B | 129 | 47.620 | -0.619 | 79.358 | 1.00 | 25.25 |
| ATOM | 4021 | O | GLY | B | 129 | 48.383 | -0.686 | 80.329 | 1.00 | 18.98 |
| ATOM | 4022 | N | MET | B | 130 | 46.317 | -0.374 | 79.474 | 1.00 | 16.04 |
| ATOM | 4023 | CA | MET | B | 130 | 45.677 | -0.161 | 80.768 | 1.00 | 19.26 |
| ATOM | 4024 | CB | MET | B | 130 | 44.301 | 0.451 | 80.519 | 1.00 | 17.94 |
| ATOM | 4025 | CG | MET | B | 130 | 44.413 | 1.728 | 79.653 | 1.00 | 22.95 |
| ATOM | 4026 | SD | MET | B | 130 | 42.873 | 2.615 | 79.307 | 1.00 | 31.83 |
| ATOM | 4027 | CE | MET | B | 130 | 41.957 | 1.358 | 78.382 | 1.00 | 20.22 |
| ATOM | 4028 | C | MET | B | 130 | 45.598 | -1.548 | 81.421 | 1.00 | 22.63 |
| ATOM | 4029 | O | MET | B | 130 | 44.546 | -2.173 | 81.486 | 1.00 | 16.24 |
| ATOM | 4030 | N | HIS | B | 131 | 46.737 | -1.999 | 81.932 | 1.00 | 18.42 |
| ATOM | 4031 | CA | HIS | B | 131 | 46.853 | -3.343 | 82.472 | 1.00 | 17.07 |
| ATOM | 4032 | CB | HIS | B | 131 | 48.323 | -3.804 | 82.341 | 1.00 | 17.61 |
| ATOM | 4033 | CG | HIS | B | 131 | 49.316 | -2.979 | 83.106 | 1.00 | 14.01 |
| ATOM | 4034 | CD2 | HIS | B | 131 | 49.138 | -1.904 | 83.915 | 1.00 | 13.47 |
| ATOM | 4035 | ND1 | HIS | B | 131 | 50.680 | -3.190 | 83.051 | 1.00 | 18.00 |
| ATOM | 4036 | CE1 | HIS | B | 131 | 51.297 | -2.281 | 83.789 | 1.00 | 15.27 |
| ATOM | 4037 | NE2 | HIS | B | 131 | 50.384 | -1.489 | 84.324 | 1.00 | 17.21 |
| ATOM | 4038 | C | HIS | B | 131 | 46.329 | -3.724 | 83.852 | 1.00 | 16.41 |
| ATOM | 4039 | O | HIS | B | 131 | 46.452 | -4.883 | 84.236 | 1.00 | 19.37 |
| ATOM | 4040 | N | HIS | B | 132 | 45.721 | -2.794 | 84.586 | 1.00 | 18.64 |
| ATOM | 4041 | CA | HIS | B | 132 | 45.241 | -3.112 | 85.936 | 1.00 | 20.87 |
| ATOM | 4042 | CB | HIS | B | 132 | 45.513 | -1.935 | 86.885 | 1.00 | 18.85 |
| ATOM | 4043 | CG | HIS | B | 132 | 46.966 | -1.686 | 87.152 | 1.00 | 20.00 |
| ATOM | 4044 | CD2 | HIS | B | 132 | 47.715 | -0.563 | 87.030 | 1.00 | 15.74 |
| ATOM | 4045 | ND1 | HIS | B | 132 | 47.810 | -2.655 | 87.659 | 1.00 | 14.72 |
| ATOM | 4046 | CE1 | HIS | B | 132 | 49.014 | -2.139 | 87.837 | 1.00 | 14.64 |
| ATOM | 4047 | NE2 | HIS | B | 132 | 48.984 | -0.872 | 87.462 | 1.00 | 14.88 |
| ATOM | 4048 | C | HIS | B | 132 | 43.778 | -3.547 | 86.136 | 1.00 | 22.83 |
| ATOM | 4049 | O | HIS | B | 132 | 43.478 | -4.298 | 87.076 | 1.00 | 17.84 |

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Figure 18-62

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4050 | N | ALA | B | 133 | 42.878 | -3.088 | 85.271 | 1.00 | 16.54 |
| ATOM | 4051 | CA | ALA | B | 133 | 41.457 | -3.396 | 85.424 | 1.00 | 19.13 |
| ATOM | 4052 | CB | ALA | B | 133 | 40.654 | -2.704 | 84.328 | 1.00 | 23.56 |
| ATOM | 4053 | C | ALA | B | 133 | 41.127 | -4.883 | 85.439 | 1.00 | 23.12 |
| ATOM | 4054 | O | ALA | B | 133 | 41.718 | -5.677 | 84.696 | 1.00 | 18.03 |
| ATOM | 4055 | N | PHE | B | 134 | 40.181 | -5.257 | 86.294 | 1.00 | 19.69 |
| ATOM | 4056 | CA | PHE | B | 134 | 39.762 | -6.649 | 86.365 | 1.00 | 19.35 |
| ATOM | 4057 | CB | PHE | B | 134 | 39.583 | -7.122 | 87.818 | 1.00 | 21.26 |
| ATOM | 4058 | CG | PHE | B | 134 | 40.837 | -7.053 | 88.646 | 1.00 | 23.41 |
| ATOM | 4059 | CD1 | PHE | B | 134 | 41.041 | -6.009 | 89.544 | 1.00 | 24.25 |
| ATOM | 4060 | CD2 | PHE | B | 134 | 41.820 | -8.027 | 88.522 | 1.00 | 22.80 |
| ATOM | 4061 | CE1 | PHE | B | 134 | 42.207 | -5.935 | 90.311 | 1.00 | 23.36 |
| ATOM | 4062 | CE2 | PHE | B | 134 | 42.997 | -7.964 | 89.283 | 1.00 | 27.74 |
| ATOM | 4063 | CZ | PHE | B | 134 | 43.190 | -6.917 | 90.178 | 1.00 | 24.05 |
| ATOM | 4064 | C | PHE | B | 134 | 38.444 | -6.816 | 85.621 | 1.00 | 18.60 |
| ATOM | 4065 | O | PHE | B | 134 | 37.815 | -5.849 | 85.196 | 1.00 | 13.82 |
| ATOM | 4066 | N | LYS | B | 135 | 38.050 | -8.064 | 85.454 | 1.00 | 19.78 |
| ATOM | 4067 | CA | LYS | B | 135 | 36.813 | -8.421 | 84.782 | 1.00 | 28.09 |
| ATOM | 4068 | CB | LYS | B | 135 | 36.501 | -9.879 | 85.125 | 1.00 | 34.06 |
| ATOM | 4069 | CG | LYS | B | 135 | 35.077 | -10.310 | 84.953 | 1.00 | 42.76 |
| ATOM | 4070 | CD | LYS | B | 135 | 34.927 | -11.745 | 85.437 | 1.00 | 48.44 |
| ATOM | 4071 | CE | LYS | B | 135 | 33.462 | -12.152 | 85.531 | 1.00 | 55.66 |
| ATOM | 4072 | NZ | LYS | B | 135 | 32.727 | -11.332 | 86.544 | 1.00 | 51.65 |
| ATOM | 4073 | C | LYS | B | 135 | 35.639 | -7.512 | 85.172 | 1.00 | 28.27 |
| ATOM | 4074 | O | LYS | B | 135 | 34.927 | -6.999 | 84.309 | 1.00 | 24.86 |
| ATOM | 4075 | N | SER | B | 136 | 35.450 | -7.292 | 86.470 | 1.00 | 29.89 |
| ATOM | 4076 | CA | SER | B | 136 | 34.331 | -6.477 | 86.933 | 1.00 | 30.86 |
| ATOM | 4077 | CB | SER | B | 136 | 33.282 | -7.388 | 87.582 | 1.00 | 31.57 |
| ATOM | 4078 | OG | SER | B | 136 | 32.916 | -8.434 | 86.698 | 1.00 | 45.10 |
| ATOM | 4079 | C | SER | B | 136 | 34.705 | -5.380 | 87.923 | 1.00 | 31.50 |
| ATOM | 4080 | O | SER | B | 136 | 33.887 | -4.997 | 88.765 | 1.00 | 24.54 |
| ATOM | 4081 | N | ARG | B | 137 | 35.920 | -4.854 | 87.835 | 1.00 | 22.63 |
| ATOM | 4082 | CA | ARG | B | 137 | 36.291 | -3.826 | 88.794 | 1.00 | 25.51 |
| ATOM | 4083 | CB | ARG | B | 137 | 36.629 | -4.486 | 90.136 | 1.00 | 29.62 |
| ATOM | 4084 | CG | ARG | B | 137 | 36.391 | -3.578 | 91.318 | 1.00 | 36.21 |
| ATOM | 4085 | CD | ARG | B | 137 | 36.874 | -4.160 | 92.631 | 1.00 | 40.79 |
| ATOM | 4086 | NE | ARG | B | 137 | 36.365 | -3.357 | 93.744 | 1.00 | 45.95 |
| ATOM | 4087 | CZ | ARG | B | 137 | 36.863 | -3.369 | 94.973 | 1.00 | 41.97 |
| ATOM | 4088 | NH1 | ARG | B | 137 | 37.897 | -4.144 | 95.263 | 1.00 | 43.42 |
| ATOM | 4089 | NH2 | ARG | B | 137 | 36.322 | -2.604 | 95.913 | 1.00 | 46.65 |
| ATOM | 4090 | C | ARG | B | 137 | 37.461 | -2.956 | 88.339 | 1.00 | 24.73 |
| ATOM | 4091 | O | ARG | B | 137 | 38.420 | -3.441 | 87.734 | 1.00 | 19.32 |
| ATOM | 4092 | N | ALA | B | 138 | 37.372 | -1.663 | 88.631 | 1.00 | 16.77 |
| ATOM | 4093 | CA | ALA | B | 138 | 38.428 | -0.733 | 88.270 | 1.00 | 18.50 |
| ATOM | 4094 | CB | ALA | B | 138 | 37.939 | 0.694 | 88.401 | 1.00 | 17.24 |
| ATOM | 4095 | C | ALA | B | 138 | 39.597 | -0.964 | 89.216 | 1.00 | 22.62 |
| ATOM | 4096 | O | ALA | B | 138 | 39.411 | -1.419 | 90.346 | 1.00 | 18.98 |
| ATOM | 4097 | N | ASN | B | 139 | 40.301 | -0.641 | 88.759 | 1.00 | 20.82 |
| ATOM | 4098 | CA | ASN | B | 139 | 41.989 | -0.828 | 89.585 | 1.00 | 25.17 |
| ATOM | 4099 | CB | ASN | B | 139 | 42.311 | -2.329 | 89.689 | 1.00 | 20.59 |
| ATOM | 4100 | CG | ASN | B | 139 | 43.556 | -2.608 | 90.511 | 1.00 | 27.70 |
| ATOM | 4101 | OD1 | ASN | B | 139 | 43.726 | -2.057 | 91.592 | 1.00 | 22.43 |
| ATOM | 4102 | ND2 | ASN | B | 139 | 44.420 | -3.487 | 90.010 | 1.00 | 24.43 |
| ATOM | 4103 | C | ASN | B | 139 | 43.176 | -0.062 | 89.020 | 1.00 | 22.37 |
| ATOM | 4104 | O | ASN | B | 139 | 43.338 | 0.038 | 87.799 | 1.00 | 17.50 |
| ATOM | 4105 | N | GLY | B | 140 | 43.984 | 0.496 | 89.920 | 1.00 | 21.67 |
| ATOM | 4106 | CA | GLY | B | 140 | 45.166 | 1.249 | 89.524 | 1.00 | 23.06 |
| ATOM | 4107 | C | GLY | B | 140 | 45.005 | 2.268 | 88.402 | 1.00 | 26.29 |
| ATOM | 4108 | O | GLY | B | 140 | 45.827 | 2.301 | 87.479 | 1.00 | 22.47 |
| ATOM | 4109 | N | PHE | B | 141 | 43.958 | 3.093 | 88.473 | 1.00 | 22.33 |
| ATOM | 4110 | CA | PHE | B | 141 | 43.694 | 4.126 | 87.461 | 1.00 | 19.01 |
| ATOM | 4111 | CB | PHE | B | 141 | 44.996 | 4.806 | 86.997 | 1.00 | 22.90 |
| ATOM | 4112 | CG | PHE | B | 141 | 45.810 | 5.433 | 88.097 | 1.00 | 23.17 |
| ATOM | 4113 | CD1 | PHE | B | 141 | 47.114 | 5.851 | 87.842 | 1.00 | 22.17 |
| ATOM | 4114 | CD2 | PHE | B | 141 | 45.281 | 5.635 | 89.366 | 1.00 | 23.40 |
| ATOM | 4115 | CE1 | PHE | B | 141 | 47.876 | 6.462 | 88.833 | 1.00 | 24.02 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-63

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4116 | CE2 | PHE | B | 141 | 46.033 | 6.244 | 90.361 | 1.00 | 23.03 |
| ATOM | 4117 | CZ | PHE | B | 141 | 47.335 | 6.658 | 90.092 | 1.00 | 25.15 |
| ATOM | 4118 | C | PHE | B | 141 | 43.029 | 3.538 | 86.214 | 1.00 | 23.69 |
| ATOM | 4119 | O | PHE | B | 141 | 42.596 | 4.283 | 85.335 | 1.00 | 18.88 |
| ATOM | 4120 | N | CYS | B | 142 | 42.962 | 2.211 | 86.122 | 1.00 | 15.03 |
| ATOM | 4121 | CA | CYS | B | 142 | 42.380 | 1.578 | 84.938 | 1.00 | 19.55 |
| ATOM | 4122 | CB | CYS | B | 142 | 43.193 | 0.336 | 84.552 | 1.00 | 20.38 |
| ATOM | 4123 | SG | CYS | B | 142 | 44.933 | 0.662 | 84.190 | 1.00 | 37.40 |
| ATOM | 4124 | C | CYS | B | 142 | 40.923 | 1.171 | 85.098 | 1.00 | 22.77 |
| ATOM | 4125 | O | CYS | B | 142 | 40.561 | 0.514 | 86.082 | 1.00 | 23.04 |
| ATOM | 4126 | N | TYR | B | 143 | 40.094 | 1.557 | 84.130 | 1.00 | 15.24 |
| ATOM | 4127 | CA | TYR | B | 143 | 38.675 | 1.194 | 84.155 | 1.00 | 21.97 |
| ATOM | 4128 | CB | TYR | B | 143 | 37.795 | 2.372 | 83.723 | 1.00 | 18.06 |
| ATOM | 4129 | CG | TYR | B | 143 | 38.016 | 3.622 | 84.535 | 1.00 | 24.34 |
| ATOM | 4130 | CD1 | TYR | B | 143 | 39.038 | 4.516 | 84.214 | 1.00 | 23.20 |
| ATOM | 4131 | CE1 | TYR | B | 143 | 39.265 | 5.658 | 84.991 | 1.00 | 27.42 |
| ATOM | 4132 | CD2 | TYR | B | 143 | 37.226 | 3.892 | 85.652 | 1.00 | 19.15 |
| ATOM | 4133 | CE2 | TYR | B | 143 | 37.441 | 5.023 | 86.432 | 1.00 | 21.92 |
| ATOM | 4134 | CZ | TYR | B | 143 | 38.458 | 5.900 | 86.099 | 1.00 | 23.94 |
| ATOM | 4135 | OH | TYR | B | 143 | 38.655 | 7.015 | 86.877 | 1.00 | 22.37 |
| ATOM | 4136 | C | TYR | B | 143 | 38.431 | 0.008 | 83.218 | 1.00 | 19.91 |
| ATOM | 4137 | O | TYR | B | 143 | 37.665 | -0.902 | 83.535 | 1.00 | 22.50 |
| ATOM | 4138 | N | ILE | B | 144 | 39.083 | 0.026 | 82.061 | 1.00 | 19.20 |
| ATOM | 4139 | CA | ILE | B | 144 | 38.938 | -1.055 | 81.082 | 1.00 | 19.68 |
| ATOM | 4140 | CB | ILE | B | 144 | 38.282 | -0.528 | 79.787 | 1.00 | 20.26 |
| ATOM | 4141 | CG2 | ILE | B | 144 | 38.151 | -1.649 | 78.760 | 1.00 | 15.37 |
| ATOM | 4142 | CG1 | ILE | B | 144 | 36.901 | 0.053 | 80.113 | 1.00 | 20.93 |
| ATOM | 4143 | CD1 | ILE | B | 144 | 36.198 | 0.697 | 78.917 | 1.00 | 23.75 |
| ATOM | 4144 | C | ILE | B | 144 | 40.320 | -1.627 | 80.774 | 1.00 | 22.78 |
| ATOM | 4145 | O | ILE | B | 144 | 41.281 | -0.873 | 80.600 | 1.00 | 22.01 |
| ATOM | 4146 | N | ASN | B | 145 | 40.422 | -2.956 | 80.723 | 1.00 | 23.18 |
| ATOM | 4147 | CA | ASN | B | 145 | 41.698 | -3.623 | 80.451 | 1.00 | 20.63 |
| ATOM | 4148 | CB | ASN | B | 145 | 41.778 | -4.935 | 81.243 | 1.00 | 17.81 |
| ATOM | 4149 | CG | ASN | B | 145 | 43.188 | -5.531 | 81.268 | 1.00 | 25.17 |
| ATOM | 4150 | OD1 | ASN | B | 145 | 43.804 | -5.742 | 80.227 | 1.00 | 23.63 |
| ATOM | 4151 | ND2 | ASN | B | 145 | 43.693 | -5.819 | 82.472 | 1.00 | 22.69 |
| ATOM | 4152 | C | ASN | B | 145 | 41.780 | -3.918 | 78.955 | 1.00 | 21.18 |
| ATOM | 4153 | O | ASN | B | 145 | 41.389 | -5.002 | 78.508 | 1.00 | 17.80 |
| ATOM | 4154 | N | ASN | B | 146 | 42.293 | -2.968 | 78.177 | 1.00 | 15.23 |
| ATOM | 4155 | CA | ASN | B | 146 | 42.367 | -3.175 | 76.733 | 1.00 | 19.71 |
| ATOM | 4156 | CB | ASN | B | 146 | 42.773 | -1.880 | 76.015 | 1.00 | 17.65 |
| ATOM | 4157 | CG | ASN | B | 146 | 44.196 | -1.458 | 76.306 | 1.00 | 19.86 |
| ATOM | 4158 | OD1 | ASN | B | 146 | 45.109 | -1.735 | 75.532 | 1.00 | 20.27 |
| ATOM | 4159 | ND2 | ASN | B | 146 | 44.395 | -0.798 | 77.435 | 1.00 | 11.85 |
| ATOM | 4160 | C | ASN | B | 146 | 43.277 | -4.342 | 76.331 | 1.00 | 19.07 |
| ATOM | 4161 | O | ASN | B | 146 | 43.030 | -4.996 | 75.328 | 1.00 | 18.61 |
| ATOM | 4162 | N | PRO | B | 147 | 44.358 | -4.598 | 77.082 | 1.00 | 17.78 |
| ATOM | 4163 | CD | PRO | B | 147 | 44.953 | -3.919 | 78.240 | 1.00 | 18.13 |
| ATOM | 4164 | CA | PRO | B | 147 | 45.197 | -5.735 | 76.678 | 1.00 | 19.98 |
| ATOM | 4165 | CB | PRO | B | 147 | 46.338 | -5.694 | 77.698 | 1.00 | 24.29 |
| ATOM | 4166 | CG | PRO | B | 147 | 46.425 | -4.201 | 78.020 | 1.00 | 26.27 |
| ATOM | 4167 | C | PRO | B | 147 | 44.377 | -7.041 | 76.757 | 1.00 | 20.91 |
| ATOM | 4168 | O | PRO | B | 147 | 44.461 | -7.892 | 75.871 | 1.00 | 17.58 |
| ATOM | 4169 | N | ALA | B | 148 | 43.568 | -7.172 | 77.809 | 1.00 | 15.81 |
| ATOM | 4170 | CA | ALA | B | 148 | 42.732 | -8.362 | 78.008 | 1.00 | 19.82 |
| ATOM | 4171 | CB | ALA | B | 148 | 42.049 | -8.312 | 79.372 | 1.00 | 17.50 |
| ATOM | 4172 | C | ALA | B | 148 | 41.683 | -8.473 | 76.903 | 1.00 | 22.58 |
| ATOM | 4173 | O | ALA | B | 148 | 41.419 | -9.567 | 76.404 | 1.00 | 18.38 |
| ATOM | 4174 | N | VAL | B | 149 | 41.080 | -7.341 | 76.540 | 1.00 | 22.48 |
| ATOM | 4175 | CA | VAL | B | 149 | 40.086 | -7.300 | 75.466 | 1.00 | 19.04 |
| ATOM | 4176 | CB | VAL | B | 149 | 39.503 | -5.877 | 75.281 | 1.00 | 18.96 |
| ATOM | 4177 | CG1 | VAL | B | 149 | 38.691 | -5.800 | 73.988 | 1.00 | 17.32 |
| ATOM | 4178 | CG2 | VAL | B | 149 | 38.621 | -5.531 | 76.462 | 1.00 | 15.33 |
| ATOM | 4179 | C | VAL | B | 149 | 40.763 | -7.709 | 74.166 | 1.00 | 22.12 |
| ATOM | 4180 | O | VAL | B | 149 | 40.240 | -8.535 | 73.421 | 1.00 | 21.83 |
| ATOM | 4181 | N | GLY | B | 150 | 41.927 | -7.120 | 73.903 | 1.00 | 19.51 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-64

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4182 | CA | GLY | B | 150 | 42.657 | -7.433 | 72.689 | 1.00 | 19.32 |
| ATOM | 4183 | C | GLY | B | 150 | 43.033 | -8.901 | 72.606 | 1.00 | 19.59 |
| ATOM | 4184 | O | GLY | B | 150 | 42.862 | -9.550 | 71.568 | 1.00 | 22.28 |
| ATOM | 4185 | N | ILE | B | 151 | 43.558 | -9.435 | 73.700 | 1.00 | 19.51 |
| ATOM | 4186 | CA | ILE | B | 151 | 43.958 | -10.834 | 73.723 | 1.00 | 23.21 |
| ATOM | 4187 | CB | ILE | B | 151 | 44.666 | -11.175 | 75.053 | 1.00 | 23.50 |
| ATOM | 4188 | CG2 | ILE | B | 151 | 44.918 | -12.679 | 75.158 | 1.00 | 20.01 |
| ATOM | 4189 | CG1 | ILE | B | 151 | 45.988 | -10.394 | 75.129 | 1.00 | 21.98 |
| ATOM | 4190 | CD1 | ILE | B | 151 | 46.716 | -10.502 | 76.457 | 1.00 | 21.24 |
| ATOM | 4191 | C | ILE | B | 151 | 42.749 | -11.741 | 73.490 | 1.00 | 28.40 |
| ATOM | 4192 | O | ILE | B | 151 | 42.832 | -12.692 | 72.706 | 1.00 | 22.96 |
| ATOM | 4193 | N | GLU | B | 152 | 41.623 | -11.450 | 74.144 | 1.00 | 27.32 |
| ATOM | 4194 | CA | GLU | B | 152 | 40.417 | -12.265 | 73.939 | 1.00 | 27.62 |
| ATOM | 4195 | CB | GLU | B | 152 | 39.294 | -11.845 | 74.886 | 1.00 | 26.46 |
| ATOM | 4196 | CG | GLU | B | 152 | 39.533 | -12.200 | 76.347 | 1.00 | 28.26 |
| ATOM | 4197 | CD | GLU | B | 152 | 39.613 | -13.708 | 76.592 | 1.00 | 31.10 |
| ATOM | 4198 | OE1 | GLU | B | 152 | 39.668 | -14.123 | 77.767 | 1.00 | 29.55 |
| ATOM | 4199 | OE2 | GLU | B | 152 | 39.626 | -14.481 | 75.617 | 1.00 | 30.51 |
| ATOM | 4200 | C | GLU | B | 152 | 39.948 | -12.125 | 72.497 | 1.00 | 30.30 |
| ATOM | 4201 | O | GLU | B | 152 | 39.463 | -13.082 | 71.893 | 1.00 | 25.58 |
| ATOM | 4202 | N | TYR | B | 153 | 40.093 | -10.923 | 71.948 | 1.00 | 26.23 |
| ATOM | 4203 | CA | TYR | B | 153 | 39.720 | -10.669 | 70.563 | 1.00 | 28.19 |
| ATOM | 4204 | CB | TYR | B | 153 | 40.082 | -9.235 | 70.190 | 1.00 | 27.94 |
| ATOM | 4205 | CG | TYR | B | 153 | 39.879 | -8.886 | 68.735 | 1.00 | 28.46 |
| ATOM | 4206 | CD1 | TYR | B | 153 | 38.618 | -8.560 | 68.240 | 1.00 | 25.69 |
| ATOM | 4207 | CE1 | TYR | B | 153 | 38.447 | -8.195 | 66.898 | 1.00 | 30.73 |
| ATOM | 4208 | CD2 | TYR | B | 153 | 40.962 | -8.847 | 67.856 | 1.00 | 24.82 |
| ATOM | 4209 | CE2 | TYR | B | 153 | 40.801 | -8.488 | 66.526 | 1.00 | 29.26 |
| ATOM | 4210 | CZ | TYR | B | 153 | 39.547 | -8.161 | 66.054 | 1.00 | 31.25 |
| ATOM | 4211 | OH | TYR | B | 153 | 39.406 | -7.803 | 64.735 | 1.00 | 34.22 |
| ATOM | 4212 | C | TYR | B | 153 | 40.513 | -11.627 | 69.674 | 1.00 | 28.11 |
| ATOM | 4213 | O | TYR | B | 153 | 39.975 | -12.248 | 68.759 | 1.00 | 22.06 |
| ATOM | 4214 | N | LEU | B | 154 | 41.810 | -11.725 | 69.944 | 1.00 | 26.77 |
| ATOM | 4215 | CA | LEU | B | 154 | 42.681 | -12.597 | 69.168 | 1.00 | 28.79 |
| ATOM | 4216 | CB | LEU | B | 154 | 44.142 | -12.386 | 69.592 | 1.00 | 28.06 |
| ATOM | 4217 | CG | LEU | B | 154 | 44.789 | -11.087 | 69.083 | 1.00 | 27.71 |
| ATOM | 4218 | CD1 | LEU | B | 154 | 46.119 | -10.860 | 69.759 | 1.00 | 34.15 |
| ATOM | 4219 | CD2 | LEU | B | 154 | 44.968 | -11.171 | 67.571 | 1.00 | 26.71 |
| ATOM | 4220 | C | LEU | B | 154 | 42.299 | -14.074 | 69.274 | 1.00 | 26.98 |
| ATOM | 4221 | O | LEU | B | 154 | 42.282 | -14.787 | 68.271 | 1.00 | 29.88 |
| ATOM | 4222 | N | ARG | B | 155 | 41.996 | -14.536 | 70.480 | 1.00 | 23.19 |
| ATOM | 4223 | CA | ARG | B | 155 | 41.622 | -15.936 | 70.669 | 1.00 | 29.47 |
| ATOM | 4224 | CB | ARG | B | 155 | 41.339 | -16.230 | 72.144 | 1.00 | 28.53 |
| ATOM | 4225 | CG | ARG | B | 155 | 42.527 | -15.965 | 73.053 | 1.00 | 35.03 |
| ATOM | 4226 | CD | ARG | B | 155 | 42.212 | -16.276 | 74.507 | 1.00 | 39.42 |
| ATOM | 4227 | NE | ARG | B | 155 | 42.165 | -17.706 | 74.792 | 1.00 | 30.99 |
| ATOM | 4228 | CZ | ARG | B | 155 | 41.869 | -18.209 | 75.986 | 1.00 | 41.33 |
| ATOM | 4229 | NH1 | ARG | B | 155 | 41.591 | -17.394 | 77.002 | 1.00 | 38.47 |
| ATOM | 4230 | NH2 | ARG | B | 155 | 41.672 | -19.523 | 76.178 | 1.00 | 40.67 |
| ATOM | 4231 | C | ARG | B | 155 | 40.393 | -16.260 | 69.832 | 1.00 | 29.07 |
| ATOM | 4232 | O | ARG | B | 155 | 40.325 | -17.311 | 69.203 | 1.00 | 25.31 |
| ATOM | 4233 | N | LYS | B | 156 | 39.419 | -15.357 | 69.828 | 1.00 | 28.99 |
| ATOM | 4234 | CA | LYS | B | 156 | 38.216 | -15.573 | 69.038 | 1.00 | 34.63 |
| ATOM | 4235 | CB | LYS | B | 156 | 37.148 | -14.534 | 69.386 | 1.00 | 36.63 |
| ATOM | 4236 | CG | LYS | B | 156 | 36.393 | -14.883 | 70.646 | 1.00 | 42.18 |
| ATOM | 4237 | CD | LYS | B | 156 | 37.292 | -14.900 | 71.868 | 1.00 | 51.38 |
| ATOM | 4238 | CE | LYS | B | 156 | 36.685 | -15.712 | 73.009 | 1.00 | 52.76 |
| ATOM | 4239 | NZ | LYS | B | 156 | 36.661 | -17.172 | 72.677 | 1.00 | 51.29 |
| ATOM | 4240 | C | LYS | B | 156 | 38.504 | -15.562 | 67.538 | 1.00 | 34.66 |
| ATOM | 4241 | O | LYS | B | 156 | 37.722 | -16.088 | 66.754 | 1.00 | 33.53 |
| ATOM | 4242 | N | LYS | B | 157 | 39.625 | -14.966 | 67.140 | 1.00 | 30.06 |
| ATOM | 4243 | CA | LYS | B | 157 | 39.996 | -14.945 | 65.734 | 1.00 | 31.36 |
| ATOM | 4244 | CB | LYS | B | 157 | 40.888 | -13.746 | 65.418 | 1.00 | 29.79 |
| ATOM | 4245 | CG | LYS | B | 157 | 40.157 | -12.426 | 65.359 | 1.00 | 31.52 |
| ATOM | 4246 | CD | LYS | B | 157 | 39.132 | -12.424 | 64.239 | 1.00 | 28.48 |
| ATOM | 4247 | CE | LYS | B | 157 | 38.395 | -11.101 | 64.171 | 1.00 | 31.90 |

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Figure 18-65

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4248 | NZ | LYS | B | 157 | 37.406 | -11.080 | 63.054 | 1.00 | 32.91 |
| ATOM | 4249 | C | LYS | B | 157 | 40.724 | -16.234 | 65.381 | 1.00 | 31.92 |
| ATOM | 4250 | O | LYS | B | 157 | 41.146 | -16.421 | 64.246 | 1.00 | 33.58 |
| ATOM | 4251 | N | GLY | B | 158 | 40.890 | -17.111 | 66.368 | 1.00 | 28.97 |
| ATOM | 4252 | CA | GLY | B | 158 | 41.546 | -18.379 | 66.112 | 1.00 | 28.98 |
| ATOM | 4253 | C | GLY | B | 158 | 42.962 | -18.569 | 66.622 | 1.00 | 33.33 |
| ATOM | 4254 | O | GLY | B | 158 | 43.503 | -19.672 | 66.522 | 1.00 | 30.58 |
| ATOM | 4255 | N | PHE | B | 159 | 43.578 | -17.521 | 67.164 | 1.00 | 32.80 |
| ATOM | 4256 | CA | PHE | B | 159 | 44.937 | -17.657 | 67.678 | 1.00 | 28.89 |
| ATOM | 4257 | CB | PHE | B | 159 | 45.560 | -16.286 | 67.934 | 1.00 | 30.33 |
| ATOM | 4258 | CG | PHE | B | 159 | 45.748 | -15.470 | 66.692 | 1.00 | 28.53 |
| ATOM | 4259 | CD1 | PHE | B | 159 | 44.682 | -14.787 | 66.121 | 1.00 | 24.58 |
| ATOM | 4260 | CD2 | PHE | B | 159 | 46.989 | -15.420 | 66.068 | 1.00 | 24.21 |
| ATOM | 4261 | CE1 | PHE | B | 159 | 44.849 | -14.066 | 64.948 | 1.00 | 25.26 |
| ATOM | 4262 | CE2 | PHE | B | 159 | 47.168 | -14.706 | 64.895 | 1.00 | 23.66 |
| ATOM | 4263 | CZ | PHE | B | 159 | 46.095 | -14.026 | 64.332 | 1.00 | 26.65 |
| ATOM | 4264 | C | PHE | B | 159 | 44.969 | -18.484 | 68.958 | 1.00 | 30.92 |
| ATOM | 4265 | O | PHE | B | 159 | 44.102 | -18.334 | 69.820 | 1.00 | 24.26 |
| ATOM | 4266 | N | LYS | B | 160 | 45.979 | -19.347 | 69.077 | 1.00 | 28.86 |
| ATOM | 4267 | CA | LYS | B | 160 | 46.123 | -20.224 | 70.237 | 1.00 | 30.27 |
| ATOM | 4268 | CB | LYS | B | 160 | 46.085 | -21.692 | 69.800 | 1.00 | 32.05 |
| ATOM | 4269 | CG | LYS | B | 160 | 44.806 | -22.117 | 69.113 | 1.00 | 41.13 |
| ATOM | 4270 | CD | LYS | B | 160 | 44.809 | -23.621 | 68.826 | 1.00 | 40.73 |
| ATOM | 4271 | CE | LYS | B | 160 | 45.945 | -24.031 | 67.904 | 1.00 | 43.16 |
| ATOM | 4272 | NZ | LYS | B | 160 | 45.812 | -23.408 | 66.554 | 1.00 | 48.69 |
| ATOM | 4273 | C | LYS | B | 160 | 47.394 | -19.997 | 71.048 | 1.00 | 28.23 |
| ATOM | 4274 | O | LYS | B | 160 | 47.552 | -20.561 | 72.130 | 1.00 | 25.29 |
| ATOM | 4275 | N | ARG | B | 161 | 48.320 | -19.206 | 70.520 | 1.00 | 28.51 |
| ATOM | 4276 | CA | ARG | B | 161 | 49.550 | -18.921 | 71.247 | 1.00 | 25.84 |
| ATOM | 4277 | CB | ARG | B | 161 | 50.724 | -19.719 | 70.667 | 1.00 | 25.33 |
| ATOM | 4278 | CG | ARG | B | 161 | 50.551 | -21.245 | 70.781 | 1.00 | 27.47 |
| ATOM | 4279 | CD | ARG | B | 161 | 51.833 | -21.985 | 70.394 | 1.00 | 32.27 |
| ATOM | 4280 | NE | ARG | B | 161 | 52.218 | -21.761 | 69.002 | 1.00 | 34.90 |
| ATOM | 4281 | CZ | ARG | B | 161 | 51.584 | -22.276 | 67.954 | 1.00 | 38.45 |
| ATOM | 4282 | NH1 | ARG | B | 161 | 50.527 | -23.056 | 68.130 | 1.00 | 38.77 |
| ATOM | 4283 | NH2 | ARG | B | 161 | 51.999 | -22.000 | 66.725 | 1.00 | 38.64 |
| ATOM | 4284 | C | ARG | B | 161 | 49.818 | -17.421 | 71.182 | 1.00 | 30.40 |
| ATOM | 4285 | O | ARG | B | 161 | 50.393 | -16.912 | 70.218 | 1.00 | 27.50 |
| ATOM | 4286 | N | ILE | B | 162 | 49.376 | -16.722 | 72.221 | 1.00 | 25.64 |
| ATOM | 4287 | CA | ILE | B | 162 | 49.515 | -15.273 | 72.303 | 1.00 | 27.44 |
| ATOM | 4288 | CB | ILE | B | 162 | 48.134 | -14.618 | 72.545 | 1.00 | 24.53 |
| ATOM | 4289 | CG2 | ILE | B | 162 | 48.249 | -13.101 | 72.473 | 1.00 | 25.49 |
| ATOM | 4290 | CG1 | ILE | B | 162 | 47.142 | -15.101 | 71.487 | 1.00 | 29.46 |
| ATOM | 4291 | CD1 | ILE | B | 162 | 45.688 | -14.707 | 71.758 | 1.00 | 31.94 |
| ATOM | 4292 | C | ILE | B | 162 | 50.465 | -14.868 | 73.429 | 1.00 | 22.68 |
| ATOM | 4293 | O | ILE | B | 162 | 50.311 | -15.302 | 74.568 | 1.00 | 24.25 |
| ATOM | 4294 | N | LEU | B | 163 | 50.454 | -14.042 | 73.100 | 1.00 | 19.49 |
| ATOM | 4295 | CA | LEU | B | 163 | 50.425 | -13.561 | 74.081 | 1.00 | 17.57 |
| ATOM | 4296 | CB | LEU | B | 163 | 53.850 | -13.686 | 73.528 | 1.00 | 20.54 |
| ATOM | 4297 | CG | LEU | B | 163 | 54.979 | -12.975 | 74.295 | 1.00 | 18.84 |
| ATOM | 4298 | CD1 | LEU | B | 163 | 55.102 | -13.538 | 75.690 | 1.00 | 20.55 |
| ATOM | 4299 | CD2 | LEU | B | 163 | 56.293 | -13.148 | 73.556 | 1.00 | 18.57 |
| ATOM | 4300 | C | LEU | B | 163 | 52.158 | -12.099 | 74.430 | 1.00 | 16.20 |
| ATOM | 4301 | O | LEU | B | 163 | 51.898 | -11.277 | 73.549 | 1.00 | 16.09 |
| ATOM | 4302 | N | TYR | B | 164 | 52.227 | -11.780 | 75.715 | 1.00 | 14.05 |
| ATOM | 4303 | CA | TYR | B | 164 | 52.027 | -10.411 | 76.191 | 1.00 | 16.21 |
| ATOM | 4304 | CB | TYR | B | 164 | 50.777 | -10.323 | 77.070 | 1.00 | 16.01 |
| ATOM | 4305 | CG | TYR | B | 164 | 50.534 | -8.948 | 77.667 | 1.00 | 15.08 |
| ATOM | 4306 | CD1 | TYR | B | 164 | 50.148 | -7.869 | 76.869 | 1.00 | 19.51 |
| ATOM | 4307 | CE1 | TYR | B | 164 | 49.948 | -6.597 | 77.418 | 1.00 | 12.88 |
| ATOM | 4308 | CD2 | TYR | B | 164 | 50.715 | -8.724 | 79.021 | 1.00 | 14.07 |
| ATOM | 4309 | CE2 | TYR | B | 164 | 50.520 | -7.463 | 79.583 | 1.00 | 13.66 |
| ATOM | 4310 | CZ | TYR | B | 164 | 50.139 | -6.407 | 78.782 | 1.00 | 14.72 |
| ATOM | 4311 | OH | TYR | B | 164 | 49.952 | -5.163 | 79.354 | 1.00 | 13.54 |
| ATOM | 4312 | C | TYR | B | 164 | 53.246 | -10.017 | 77.018 | 1.00 | 19.14 |
| ATOM | 4313 | O | TYR | B | 164 | 53.539 | -10.642 | 78.036 | 1.00 | 26.51 |

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Figure 18-66

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4314 | N | ILE | B | 165 | 53.964 | -8.992 | 76.573 | 1.00 | 22.40 |
| ATOM | 4315 | CA | ILE | B | 165 | 55.148 | -8.518 | 77.285 | 1.00 | 17.72 |
| ATOM | 4316 | CB | ILE | B | 165 | 56.352 | -8.465 | 76.343 | 1.00 | 22.51 |
| ATOM | 4317 | CG2 | ILE | B | 165 | 57.582 | -7.902 | 77.079 | 1.00 | 16.36 |
| ATOM | 4318 | CG1 | ILE | B | 165 | 56.632 | -9.880 | 75.818 | 1.00 | 19.82 |
| ATOM | 4319 | CD1 | ILE | B | 165 | 57.721 | -9.942 | 74.742 | 1.00 | 21.74 |
| ATOM | 4320 | C | ILE | B | 165 | 54.851 | -7.126 | 77.850 | 1.00 | 22.54 |
| ATOM | 4321 | O | ILE | B | 165 | 54.478 | -6.223 | 77.111 | 1.00 | 16.60 |
| ATOM | 4322 | N | ASP | B | 166 | 55.046 | -6.961 | 79.156 | 1.00 | 15.78 |
| ATOM | 4323 | CA | ASP | B | 166 | 54.740 | -5.704 | 79.840 | 1.00 | 20.62 |
| ATOM | 4324 | CB | ASP | B | 166 | 53.719 | -5.996 | 80.949 | 1.00 | 17.57 |
| ATOM | 4325 | CG | ASP | B | 166 | 53.063 | -4.742 | 81.486 | 1.00 | 25.39 |
| ATOM | 4326 | OD1 | ASP | B | 166 | 53.779 | -3.859 | 82.003 | 1.00 | 19.68 |
| ATOM | 4327 | OD2 | ASP | B | 166 | 51.824 | -4.637 | 81.377 | 1.00 | 29.22 |
| ATOM | 4328 | C | ASP | B | 166 | 55.976 | -5.002 | 80.423 | 1.00 | 19.01 |
| ATOM | 4329 | O | ASP | B | 166 | 56.509 | -5.412 | 81.456 | 1.00 | 19.74 |
| ATOM | 4330 | N | LEU | B | 167 | 56.414 | -3.923 | 79.775 | 1.00 | 17.88 |
| ATOM | 4331 | CA | LEU | B | 167 | 57.598 | -3.211 | 80.235 | 1.00 | 14.99 |
| ATOM | 4332 | CB | LEU | B | 167 | 58.412 | -2.710 | 79.044 | 1.00 | 19.22 |
| ATOM | 4333 | CG | LEU | B | 167 | 58.871 | -3.799 | 78.069 | 1.00 | 22.68 |
| ATOM | 4334 | CD1 | LEU | B | 167 | 59.835 | -3.179 | 77.074 | 1.00 | 25.35 |
| ATOM | 4335 | CD2 | LEU | B | 167 | 59.570 | -4.943 | 78.808 | 1.00 | 17.54 |
| ATOM | 4336 | C | LEU | B | 167 | 57.284 | -2.059 | 81.183 | 1.00 | 17.49 |
| ATOM | 4337 | O | LEU | B | 167 | 58.189 | -1.359 | 81.639 | 1.00 | 13.39 |
| ATOM | 4338 | N | ASP | B | 168 | 56.003 | -1.878 | 81.479 | 1.00 | 20.03 |
| ATOM | 4339 | CA | ASP | B | 168 | 55.549 | -0.848 | 82.412 | 1.00 | 21.98 |
| ATOM | 4340 | CB | ASP | B | 168 | 54.030 | -0.955 | 82.597 | 1.00 | 21.21 |
| ATOM | 4341 | CG | ASP | B | 168 | 53.453 | 0.186 | 83.428 | 1.00 | 24.92 |
| ATOM | 4342 | C | ASP | B | 168 | 56.241 | -1.139 | 83.753 | 1.00 | 22.98 |
| ATOM | 4343 | O | ASP | B | 168 | 56.447 | -2.304 | 84.091 | 1.00 | 18.36 |
| ATOM | 4344 | OD1 | ASP | B | 168 | 52.849 | 1.099 | 82.825 | 1.00 | 22.03 |
| ATOM | 4345 | OD2 | ASP | B | 168 | 53.606 | 0.189 | 84.676 | 1.00 | 18.43 |
| ATOM | 4346 | N | ALA | B | 169 | 56.581 | -0.095 | 84.514 | 1.00 | 15.46 |
| ATOM | 4347 | CA | ALA | B | 169 | 57.263 | -0.268 | 85.807 | 1.00 | 18.73 |
| ATOM | 4348 | CB | ALA | B | 169 | 57.764 | 1.084 | 86.323 | 1.00 | 11.98 |
| ATOM | 4349 | C | ALA | B | 169 | 56.400 | -0.940 | 86.886 | 1.00 | 21.82 |
| ATOM | 4350 | O | ALA | B | 169 | 56.886 | -1.262 | 87.980 | 1.00 | 22.51 |
| ATOM | 4351 | N | HIS | B | 170 | 55.120 | -1.134 | 86.600 | 1.00 | 18.75 |
| ATOM | 4352 | CA | HIS | B | 170 | 54.238 | -1.776 | 87.570 | 1.00 | 22.70 |
| ATOM | 4353 | C | HIS | B | 170 | 53.716 | -3.096 | 87.015 | 1.00 | 22.11 |
| ATOM | 4354 | O | HIS | B | 170 | 53.536 | -3.244 | 85.809 | 1.00 | 21.94 |
| ATOM | 4355 | CB | HIS | B | 170 | 53.050 | -0.867 | 87.927 | 1.00 | 21.28 |
| ATOM | 4356 | CG | HIS | B | 170 | 53.449 | 0.475 | 88.460 | 1.00 | 18.89 |
| ATOM | 4357 | ND1 | HIS | B | 170 | 53.695 | 1.539 | 87.626 | 1.00 | 19.13 |
| ATOM | 4358 | CE1 | HIS | B | 170 | 54.046 | 2.539 | 88.412 | 1.00 | 19.41 |
| ATOM | 4359 | CD2 | HIS | B | 170 | 53.660 | 0.854 | 89.746 | 1.00 | 19.02 |
| ATOM | 4360 | NE2 | HIS | B | 170 | 54.042 | 2.174 | 89.710 | 1.00 | 20.45 |
| ATOM | 4361 | N | HIS | B | 171 | 53.474 | -4.047 | 87.907 | 1.00 | 19.20 |
| ATOM | 4362 | CA | HIS | B | 171 | 52.961 | -5.352 | 87.519 | 1.00 | 21.20 |
| ATOM | 4363 | CB | HIS | B | 171 | 52.964 | -6.284 | 88.722 | 1.00 | 22.00 |
| ATOM | 4364 | CG | HIS | B | 171 | 52.541 | -7.683 | 88.400 | 1.00 | 24.64 |
| ATOM | 4365 | CD2 | HIS | B | 171 | 53.056 | -8.594 | 87.540 | 1.00 | 19.19 |
| ATOM | 4366 | ND1 | HIS | B | 171 | 51.441 | -8.279 | 88.979 | 1.00 | 25.71 |
| ATOM | 4367 | CE1 | HIS | B | 171 | 51.295 | -9.497 | 88.487 | 1.00 | 25.30 |
| ATOM | 4368 | NE2 | HIS | B | 171 | 52.261 | -9.713 | 87.612 | 1.00 | 24.71 |
| ATOM | 4369 | C | HIS | B | 171 | 51.549 | -5.306 | 86.943 | 1.00 | 23.91 |
| ATOM | 4370 | O | HIS | B | 171 | 50.677 | -4.620 | 87.479 | 1.00 | 18.93 |
| ATOM | 4371 | N | CYS | B | 172 | 51.332 | -6.062 | 85.865 | 1.00 | 15.36 |
| ATOM | 4372 | CA | CYS | B | 172 | 50.036 | -6.141 | 85.207 | 1.00 | 20.03 |
| ATOM | 4373 | CB | CYS | B | 172 | 50.240 | -6.534 | 83.732 | 1.00 | 22.46 |
| ATOM | 4374 | SG | CYS | B | 172 | 51.259 | -8.030 | 83.419 | 1.00 | 23.49 |
| ATOM | 4375 | C | CYS | B | 172 | 49.110 | -7.146 | 85.913 | 1.00 | 18.05 |
| ATOM | 4376 | O | CYS | B | 172 | 48.712 | -8.151 | 85.327 | 1.00 | 18.23 |
| ATOM | 4377 | N | ASP | B | 173 | 48.767 | -6.871 | 87.170 | 1.00 | 16.78 |
| ATOM | 4378 | CA | ASP | B | 173 | 47.909 | -7.776 | 87.928 | 1.00 | 18.81 |
| ATOM | 4379 | CB | ASP | B | 173 | 47.638 | -7.236 | 89.344 | 1.00 | 20.39 |

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Figure 18-67

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4380 | CG | ASP | B | 173 | 46.961 | -5.871 | 89.354 | 1.00 | 23.40 |
| ATOM | 4381 | OD1 | ASP | B | 173 | 46.564 | -5.435 | 90.455 | 1.00 | 18.64 |
| ATOM | 4382 | OD2 | ASP | B | 173 | 46.834 | -5.231 | 88.291 | 1.00 | 19.24 |
| ATOM | 4383 | C | ASP | B | 173 | 46.595 | -8.116 | 87.219 | 1.00 | 17.46 |
| ATOM | 4384 | O | ASP | B | 173 | 46.162 | -9.272 | 87.224 | 1.00 | 15.53 |
| ATOM | 4385 | N | GLY | B | 174 | 45.978 | -7.130 | 86.580 | 1.00 | 13.46 |
| ATOM | 4386 | CA | GLY | B | 174 | 44.733 | -7.391 | 85.876 | 1.00 | 18.18 |
| ATOM | 4387 | C | GLY | B | 174 | 44.904 | -8.392 | 84.741 | 1.00 | 17.85 |
| ATOM | 4388 | O | GLY | B | 174 | 44.104 | -9.316 | 84.583 | 1.00 | 18.27 |
| ATOM | 4389 | N | VAL | B | 175 | 45.951 | -8.214 | 83.943 | 1.00 | 16.14 |
| ATOM | 4390 | CA | VAL | B | 175 | 46.206 | -9.111 | 82.829 | 1.00 | 17.00 |
| ATOM | 4391 | CB | VAL | B | 175 | 47.305 | -8.552 | 81.902 | 1.00 | 27.22 |
| ATOM | 4392 | CG1 | VAL | B | 175 | 47.533 | -9.507 | 80.731 | 1.00 | 19.75 |
| ATOM | 4393 | CG2 | VAL | B | 175 | 46.896 | -7.169 | 81.396 | 1.00 | 18.66 |
| ATOM | 4394 | C | VAL | B | 175 | 46.635 | -10.486 | 83.324 | 1.00 | 22.82 |
| ATOM | 4395 | O | VAL | B | 175 | 46.255 | -11.503 | 82.754 | 1.00 | 18.06 |
| ATOM | 4396 | N | GLN | B | 176 | 47.439 | -10.520 | 84.378 | 1.00 | 21.67 |
| ATOM | 4397 | CA | GLN | B | 176 | 47.889 | -11.798 | 84.911 | 1.00 | 21.55 |
| ATOM | 4398 | CB | GLN | B | 176 | 48.824 | -11.602 | 86.105 | 1.00 | 19.68 |
| ATOM | 4399 | CG | GLN | B | 176 | 49.088 | -12.905 | 86.862 | 1.00 | 20.17 |
| ATOM | 4400 | CD | GLN | B | 176 | 50.066 | -12.759 | 87.996 | 1.00 | 25.42 |
| ATOM | 4401 | OE1 | GLN | B | 176 | 51.243 | -12.442 | 87.786 | 1.00 | 21.56 |
| ATOM | 4402 | NE2 | GLN | B | 176 | 49.592 | -13.000 | 89.217 | 1.00 | 20.18 |
| ATOM | 4403 | C | GLN | B | 176 | 46.689 | -12.630 | 85.348 | 1.00 | 24.78 |
| ATOM | 4404 | O | GLN | B | 176 | 46.618 | -13.817 | 85.057 | 1.00 | 22.91 |
| ATOM | 4405 | N | GLU | B | 177 | 45.751 | -12.007 | 86.051 | 1.00 | 23.69 |
| ATOM | 4406 | CA | GLU | B | 177 | 44.571 | -12.727 | 86.523 | 1.00 | 27.01 |
| ATOM | 4407 | CB | GLU | B | 177 | 43.703 | -11.825 | 87.394 | 1.00 | 24.73 |
| ATOM | 4408 | CG | GLU | B | 177 | 42.633 | -12.581 | 88.138 | 1.00 | 37.46 |
| ATOM | 4409 | CD | GLU | B | 177 | 41.767 | -11.676 | 88.987 | 1.00 | 42.48 |
| ATOM | 4410 | OE1 | GLU | B | 177 | 40.875 | -11.002 | 88.432 | 1.00 | 44.35 |
| ATOM | 4411 | OE2 | GLU | B | 177 | 41.993 | -11.627 | 90.213 | 1.00 | 45.63 |
| ATOM | 4412 | C | GLU | B | 177 | 43.732 | -13.247 | 85.370 | 1.00 | 26.56 |
| ATOM | 4413 | O | GLU | B | 177 | 43.240 | -14.375 | 85.408 | 1.00 | 27.71 |
| ATOM | 4414 | N | ALA | B | 178 | 43.573 | -12.418 | 84.344 | 1.00 | 24.58 |
| ATOM | 4415 | CA | ALA | B | 178 | 42.776 | -12.775 | 83.174 | 1.00 | 25.86 |
| ATOM | 4416 | CB | ALA | B | 178 | 42.778 | -11.628 | 82.171 | 1.00 | 24.20 |
| ATOM | 4417 | C | ALA | B | 178 | 43.231 | -14.054 | 82.485 | 1.00 | 25.72 |
| ATOM | 4418 | O | ALA | B | 178 | 42.406 | -14.838 | 82.036 | 1.00 | 22.38 |
| ATOM | 4419 | N | PHE | B | 179 | 44.535 | -14.282 | 82.395 | 1.00 | 27.19 |
| ATOM | 4420 | CA | PHE | B | 179 | 44.990 | -15.489 | 81.703 | 1.00 | 27.05 |
| ATOM | 4421 | CB | PHE | B | 179 | 45.714 | -15.086 | 80.418 | 1.00 | 25.22 |
| ATOM | 4422 | CG | PHE | B | 179 | 44.992 | -14.020 | 79.644 | 1.00 | 20.36 |
| ATOM | 4423 | CD1 | PHE | B | 179 | 45.387 | -12.687 | 79.735 | 1.00 | 25.23 |
| ATOM | 4424 | CD2 | PHE | B | 179 | 43.860 | -14.332 | 78.902 | 1.00 | 19.22 |
| ATOM | 4425 | CE1 | PHE | B | 179 | 44.659 | -11.677 | 79.102 | 1.00 | 19.25 |
| ATOM | 4426 | CE2 | PHE | B | 179 | 43.128 | -13.315 | 78.272 | 1.00 | 20.65 |
| ATOM | 4427 | CZ | PHE | B | 179 | 43.528 | -12.001 | 78.374 | 1.00 | 25.64 |
| ATOM | 4428 | C | PHE | B | 179 | 45.866 | -16.398 | 82.556 | 1.00 | 23.50 |
| ATOM | 4429 | O | PHE | B | 179 | 46.652 | -17.182 | 82.038 | 1.00 | 18.26 |
| ATOM | 4430 | N | TYR | B | 180 | 45.689 | -16.313 | 83.868 | 1.00 | 23.24 |
| ATOM | 4431 | CA | TYR | B | 180 | 46.479 | -17.106 | 84.799 | 1.00 | 26.76 |
| ATOM | 4432 | CB | TYR | B | 180 | 46.150 | -16.665 | 86.231 | 1.00 | 25.72 |
| ATOM | 4433 | CG | TYR | B | 180 | 47.226 | -16.969 | 87.247 | 1.00 | 29.66 |
| ATOM | 4434 | CD1 | TYR | B | 180 | 47.037 | -17.942 | 88.237 | 1.00 | 27.07 |
| ATOM | 4435 | CE1 | TYR | B | 180 | 48.039 | -18.222 | 89.170 | 1.00 | 30.08 |
| ATOM | 4436 | CD2 | TYR | B | 180 | 48.444 | -16.283 | 87.216 | 1.00 | 29.68 |
| ATOM | 4437 | CE2 | TYR | B | 180 | 49.451 | -16.552 | 88.139 | 1.00 | 30.99 |
| ATOM | 4438 | CZ | TYR | B | 180 | 49.248 | -17.521 | 89.112 | 1.00 | 33.16 |
| ATOM | 4439 | OH | TYR | B | 180 | 50.262 | -17.791 | 90.006 | 1.00 | 28.47 |
| ATOM | 4440 | C | TYR | B | 180 | 46.256 | -18.619 | 84.649 | 1.00 | 29.13 |
| ATOM | 4441 | O | TYR | B | 180 | 47.163 | -19.416 | 84.922 | 1.00 | 23.43 |
| ATOM | 4442 | N | ASP | B | 181 | 45.073 | -19.021 | 84.190 | 1.00 | 25.67 |
| ATOM | 4443 | CA | ASP | B | 181 | 44.784 | -20.445 | 84.075 | 1.00 | 28.28 |
| ATOM | 4444 | CB | ASP | B | 181 | 43.446 | -20.759 | 84.757 | 1.00 | 32.13 |
| ATOM | 4445 | CG | ASP | B | 181 | 42.247 | -20.410 | 83.890 | 1.00 | 36.12 |

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Figure 18-68

| | | | | | | | |
|------|------|---------------|--------|---------|--------|------|-------|
| ATOM | 4446 | OD1 ASP B 181 | 42.202 | -19.300 | 83.329 | 1.00 | 41.04 |
| ATOM | 4447 | OD2 ASP B 181 | 41.334 | -21.249 | 83.782 | 1.00 | 44.36 |
| ATOM | 4448 | C ASP B 181 | 44.773 | -21.018 | 82.664 | 1.00 | 32.41 |
| ATOM | 4449 | O ASP B 181 | 44.246 | -22.115 | 82.444 | 1.00 | 31.67 |
| ATOM | 4450 | N THR B 182 | 45.345 | -20.302 | 81.702 | 1.00 | 29.24 |
| ATOM | 4451 | CA THR B 182 | 45.363 | -20.823 | 80.340 | 1.00 | 30.57 |
| ATOM | 4452 | CB THR B 182 | 44.468 | -20.008 | 79.397 | 1.00 | 30.03 |
| ATOM | 4453 | OG1 THR B 182 | 44.516 | -20.598 | 78.095 | 1.00 | 28.22 |
| ATOM | 4454 | CG2 THR B 182 | 44.947 | -18.561 | 79.310 | 1.00 | 26.55 |
| ATOM | 4455 | C THR B 182 | 46.759 | -20.870 | 79.740 | 1.00 | 32.31 |
| ATOM | 4456 | O THR B 182 | 47.591 | -20.007 | 80.008 | 1.00 | 27.27 |
| ATOM | 4457 | N ASP B 183 | 46.999 | -21.878 | 78.909 | 1.00 | 29.94 |
| ATOM | 4458 | CA ASP B 183 | 48.296 | -22.049 | 78.273 | 1.00 | 31.40 |
| ATOM | 4459 | CB ASP B 183 | 48.648 | -23.536 | 78.228 | 1.00 | 33.36 |
| ATOM | 4460 | CG ASP B 183 | 47.718 | -24.319 | 77.328 | 1.00 | 33.33 |
| ATOM | 4461 | OD1 ASP B 183 | 46.513 | -23.988 | 77.287 | 1.00 | 28.06 |
| ATOM | 4462 | OD2 ASP B 183 | 48.186 | -25.271 | 76.675 | 1.00 | 38.19 |
| ATOM | 4463 | C ASP B 183 | 48.321 | -21.462 | 76.864 | 1.00 | 31.14 |
| ATOM | 4464 | O ASP B 183 | 49.332 | -21.557 | 76.168 | 1.00 | 28.74 |
| ATOM | 4465 | N GLN B 184 | 47.217 | -20.852 | 76.446 | 1.00 | 25.34 |
| ATOM | 4466 | CA GLN B 184 | 47.151 | -20.251 | 75.118 | 1.00 | 28.59 |
| ATOM | 4467 | CB GLN B 184 | 45.712 | -20.256 | 74.581 | 1.00 | 26.84 |
| ATOM | 4468 | CG GLN B 184 | 45.060 | -21.632 | 74.529 | 1.00 | 34.86 |
| ATOM | 4469 | CD GLN B 184 | 43.760 | -21.647 | 73.736 | 1.00 | 32.27 |
| ATOM | 4470 | OE1 GLN B 184 | 42.897 | -20.789 | 73.912 | 1.00 | 35.43 |
| ATOM | 4471 | NE2 GLN B 184 | 43.611 | -22.641 | 72.870 | 1.00 | 28.92 |
| ATOM | 4472 | C GLN B 184 | 47.672 | -18.817 | 75.175 | 1.00 | 27.28 |
| ATOM | 4473 | O GLN B 184 | 47.871 | -18.171 | 74.148 | 1.00 | 29.70 |
| ATOM | 4474 | N VAL B 185 | 47.900 | -18.325 | 76.386 | 1.00 | 27.64 |
| ATOM | 4475 | CA VAL B 185 | 48.400 | -16.972 | 76.575 | 1.00 | 26.26 |
| ATOM | 4476 | CB VAL B 185 | 47.304 | -16.039 | 77.145 | 1.00 | 22.85 |
| ATOM | 4477 | CG1 VAL B 185 | 47.879 | -14.642 | 77.395 | 1.00 | 23.10 |
| ATOM | 4478 | CG2 VAL B 185 | 46.136 | -15.967 | 76.191 | 1.00 | 21.67 |
| ATOM | 4479 | C VAL B 185 | 49.570 | -16.964 | 77.547 | 1.00 | 27.01 |
| ATOM | 4480 | O VAL B 185 | 49.456 | -17.469 | 78.663 | 1.00 | 23.75 |
| ATOM | 4481 | N PHE B 186 | 50.696 | -16.403 | 77.115 | 1.00 | 22.02 |
| ATOM | 4482 | CA PHE B 186 | 51.868 | -16.301 | 77.978 | 1.00 | 21.83 |
| ATOM | 4483 | CB PHE B 186 | 53.142 | -16.763 | 77.252 | 1.00 | 17.02 |
| ATOM | 4484 | CG PHE B 186 | 54.336 | -16.921 | 78.170 | 1.00 | 24.84 |
| ATOM | 4485 | CD1 PHE B 186 | 54.756 | -18.189 | 78.580 | 1.00 | 22.70 |
| ATOM | 4486 | CD2 PHE B 186 | 55.004 | -15.805 | 78.670 | 1.00 | 20.26 |
| ATOM | 4487 | CE1 PHE B 186 | 55.819 | -18.338 | 79.471 | 1.00 | 21.47 |
| ATOM | 4488 | CE2 PHE B 186 | 56.071 | -15.941 | 79.563 | 1.00 | 20.01 |
| ATOM | 4489 | CZ PHE B 186 | 56.481 | -17.206 | 79.968 | 1.00 | 17.84 |
| ATOM | 4490 | C PHE B 186 | 52.032 | -14.827 | 78.368 | 1.00 | 18.12 |
| ATOM | 4491 | O PHE B 186 | 52.038 | -13.946 | 77.508 | 1.00 | 15.92 |
| ATOM | 4492 | N VAL B 187 | 52.161 | -14.565 | 79.661 | 1.00 | 18.06 |
| ATOM | 4493 | CA VAL B 187 | 52.348 | -13.208 | 80.153 | 1.00 | 17.67 |
| ATOM | 4494 | CB VAL B 187 | 51.282 | -12.839 | 81.225 | 1.00 | 22.85 |
| ATOM | 4495 | CG1 VAL B 187 | 51.608 | -11.473 | 81.840 | 1.00 | 24.08 |
| ATOM | 4496 | CG2 VAL B 187 | 49.882 | -12.808 | 80.598 | 1.00 | 18.82 |
| ATOM | 4497 | C VAL B 187 | 53.735 | -13.060 | 80.788 | 1.00 | 18.32 |
| ATOM | 4498 | O VAL B 187 | 54.092 | -13.807 | 81.707 | 1.00 | 18.82 |
| ATOM | 4499 | N LEU B 188 | 54.503 | -12.103 | 80.282 | 1.00 | 14.70 |
| ATOM | 4500 | CA LEU B 188 | 55.832 | -11.789 | 80.798 | 1.00 | 18.84 |
| ATOM | 4501 | CB LEU B 188 | 56.900 | -11.948 | 79.716 | 1.00 | 18.64 |
| ATOM | 4502 | CG LEU B 188 | 58.230 | -11.277 | 80.082 | 1.00 | 21.23 |
| ATOM | 4503 | CD1 LEU B 188 | 58.769 | -11.832 | 81.395 | 1.00 | 18.55 |
| ATOM | 4504 | CD2 LEU B 188 | 59.227 | -11.489 | 78.957 | 1.00 | 20.49 |
| ATOM | 4505 | C LEU B 188 | 55.836 | -10.339 | 81.280 | 1.00 | 22.14 |
| ATOM | 4506 | O LEU B 188 | 55.527 | -9.410 | 80.517 | 1.00 | 19.96 |
| ATOM | 4507 | N SER B 189 | 56.187 | -10.133 | 82.540 | 1.00 | 21.08 |
| ATOM | 4508 | CA SER B 189 | 56.203 | -8.782 | 83.061 | 1.00 | 21.85 |
| ATOM | 4509 | CB SER B 189 | 54.956 | -8.543 | 83.908 | 1.00 | 25.95 |
| ATOM | 4510 | OG SER B 189 | 54.988 | -7.252 | 84.475 | 1.00 | 21.91 |
| ATOM | 4511 | C SER B 189 | 57.423 | -8.420 | 83.883 | 1.00 | 23.62 |

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Figure 18-69

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 4512 | O | SER B 189 | 57.829 | -9.174 | 84.766 | 1.00 | 18.61 |
| ATOM | 4513 | N | LEU B 190 | 58.020 | -7.269 | 83.569 | 1.00 | 20.83 |
| ATOM | 4514 | CA | LEU B 190 | 59.149 | -6.767 | 84.347 | 1.00 | 21.85 |
| ATOM | 4515 | CB | LEU B 190 | 60.278 | -6.226 | 83.473 | 1.00 | 22.85 |
| ATOM | 4516 | CG | LEU B 190 | 60.964 | -7.089 | 82.413 | 1.00 | 32.59 |
| ATOM | 4517 | CD1 | LEU B 190 | 62.337 | -6.479 | 82.140 | 1.00 | 29.27 |
| ATOM | 4518 | CD2 | LEU B 190 | 61.136 | -8.511 | 82.979 | 1.00 | 31.88 |
| ATOM | 4519 | C | LEU B 190 | 58.505 | -5.613 | 85.085 | 1.00 | 21.28 |
| ATOM | 4520 | O | LEU B 190 | 57.695 | -4.897 | 84.501 | 1.00 | 15.72 |
| ATOM | 4521 | N | HIS B 191 | 58.857 | -5.421 | 86.351 | 1.00 | 18.16 |
| ATOM | 4522 | CA | HIS B 191 | 58.249 | -4.357 | 87.145 | 1.00 | 17.46 |
| ATOM | 4523 | CB | HIS B 191 | 56.759 | -4.690 | 87.369 | 1.00 | 16.00 |
| ATOM | 4524 | CG | HIS B 191 | 56.517 | -6.085 | 87.880 | 1.00 | 22.14 |
| ATOM | 4525 | CD2 | HIS B 191 | 56.341 | -6.551 | 89.143 | 1.00 | 12.25 |
| ATOM | 4526 | ND1 | HIS B 191 | 56.372 | -7.179 | 87.049 | 1.00 | 18.02 |
| ATOM | 4527 | CE1 | HIS B 191 | 56.119 | -8.256 | 87.775 | 1.00 | 8.17 |
| ATOM | 4528 | NE2 | HIS B 191 | 56.094 | -7.902 | 89.049 | 1.00 | 19.79 |
| ATOM | 4529 | C | HIS B 191 | 58.945 | -4.197 | 88.484 | 1.00 | 17.41 |
| ATOM | 4530 | O | HIS B 191 | 59.769 | -5.029 | 88.867 | 1.00 | 18.74 |
| ATOM | 4531 | N | GLN B 192 | 58.618 | -3.114 | 89.182 | 1.00 | 18.20 |
| ATOM | 4532 | CA | GLN B 192 | 59.173 | -2.854 | 90.502 | 1.00 | 18.41 |
| ATOM | 4533 | CB | GLN B 192 | 58.690 | -1.500 | 91.034 | 1.00 | 20.71 |
| ATOM | 4534 | CG | GLN B 192 | 58.871 | -0.334 | 90.072 | 1.00 | 21.49 |
| ATOM | 4535 | CD | GLN B 192 | 58.226 | 0.930 | 90.594 | 1.00 | 20.65 |
| ATOM | 4536 | OE1 | GLN B 192 | 58.775 | 1.615 | 91.459 | 1.00 | 21.52 |
| ATOM | 4537 | NE2 | GLN B 192 | 57.029 | 1.226 | 90.098 | 1.00 | 15.10 |
| ATOM | 4538 | C | GLN B 192 | 58.608 | -3.945 | 91.395 | 1.00 | 17.55 |
| ATOM | 4539 | O | GLN B 192 | 57.415 | -4.256 | 91.320 | 1.00 | 17.48 |
| ATOM | 4540 | N | SER B 193 | 59.447 | -4.522 | 92.240 | 1.00 | 15.71 |
| ATOM | 4541 | CA | SER B 193 | 58.986 | -5.574 | 93.143 | 1.00 | 20.58 |
| ATOM | 4542 | CB | SER B 193 | 60.093 | -5.963 | 94.120 | 1.00 | 20.71 |
| ATOM | 4543 | OG | SER B 193 | 59.571 | -6.804 | 95.138 | 1.00 | 22.55 |
| ATOM | 4544 | C | SER B 193 | 57.774 | -5.112 | 93.947 | 1.00 | 21.81 |
| ATOM | 4545 | O | SER B 193 | 57.769 | -4.003 | 94.486 | 1.00 | 20.82 |
| ATOM | 4546 | N | PRO B 194 | 56.745 | -5.967 | 94.063 | 1.00 | 21.80 |
| ATOM | 4547 | CD | PRO B 194 | 56.648 | -7.331 | 93.524 | 1.00 | 24.27 |
| ATOM | 4548 | CA | PRO B 194 | 55.524 | -5.643 | 94.812 | 1.00 | 23.58 |
| ATOM | 4549 | CB | PRO B 194 | 54.678 | -6.909 | 94.642 | 1.00 | 22.98 |
| ATOM | 4550 | CG | PRO B 194 | 55.168 | -7.458 | 93.317 | 1.00 | 26.35 |
| ATOM | 4551 | C | PRO B 194 | 55.841 | -5.366 | 96.283 | 1.00 | 25.79 |
| ATOM | 4552 | O | PRO B 194 | 55.009 | -4.831 | 97.022 | 1.00 | 27.26 |
| ATOM | 4553 | N | GLU B 195 | 57.045 | -5.736 | 96.710 | 1.00 | 23.20 |
| ATOM | 4554 | CA | GLU B 195 | 57.428 | -5.514 | 98.093 | 1.00 | 29.56 |
| ATOM | 4555 | CB | GLU B 195 | 58.816 | -6.090 | 98.379 | 1.00 | 32.38 |
| ATOM | 4556 | CG | GLU B 195 | 58.940 | -7.567 | 98.049 | 1.00 | 45.25 |
| ATOM | 4557 | CD | GLU B 195 | 60.206 | -8.189 | 98.613 | 1.00 | 50.44 |
| ATOM | 4558 | OE1 | GLU B 195 | 61.290 | -7.580 | 98.471 | 1.00 | 50.51 |
| ATOM | 4559 | OE2 | GLU B 195 | 60.118 | -9.297 | 99.184 | 1.00 | 49.77 |
| ATOM | 4560 | C | GLU B 195 | 57.414 | -4.035 | 98.425 | 1.00 | 25.11 |
| ATOM | 4561 | O | GLU B 195 | 57.095 | -3.659 | 99.551 | 1.00 | 29.05 |
| ATOM | 4562 | N | TYR B 196 | 57.729 | -3.191 | 97.445 | 1.00 | 22.90 |
| ATOM | 4563 | CA | TYR B 196 | 57.743 | -1.750 | 97.696 | 1.00 | 22.46 |
| ATOM | 4564 | CB | TYR B 196 | 59.188 | -1.223 | 97.668 | 1.00 | 22.72 |
| ATOM | 4565 | CG | TYR B 196 | 59.855 | -1.234 | 96.301 | 1.00 | 24.17 |
| ATOM | 4566 | CD1 | TYR B 196 | 59.639 | -0.203 | 95.385 | 1.00 | 20.87 |
| ATOM | 4567 | CE1 | TYR B 196 | 60.229 | -0.222 | 94.118 | 1.00 | 18.31 |
| ATOM | 4568 | CD2 | TYR B 196 | 60.684 | -2.289 | 95.916 | 1.00 | 24.63 |
| ATOM | 4569 | CE2 | TYR B 196 | 61.276 | -2.318 | 94.648 | 1.00 | 24.39 |
| ATOM | 4570 | CZ | TYR B 196 | 61.042 | -1.284 | 93.756 | 1.00 | 23.01 |
| ATOM | 4571 | OH | TYR B 196 | 61.592 | -1.328 | 92.492 | 1.00 | 19.86 |
| ATOM | 4572 | C | TYR B 196 | 56.896 | -0.938 | 96.725 | 1.00 | 23.54 |
| ATOM | 4573 | O | TYR B 196 | 56.779 | 0.275 | 96.869 | 1.00 | 17.53 |
| ATOM | 4574 | N | ALA B 197 | 56.293 | -1.589 | 95.740 | 1.00 | 22.11 |
| ATOM | 4575 | CA | ALA B 197 | 55.503 | -0.829 | 94.779 | 1.00 | 24.28 |
| ATOM | 4576 | CB | ALA B 197 | 56.310 | -0.616 | 93.513 | 1.00 | 23.03 |
| ATOM | 4577 | C | ALA B 197 | 54.153 | -1.412 | 94.413 | 1.00 | 22.80 |

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Figure 18-70

| | | | | | | | | |
|------|------|-----|-----------|--------|---------|--------|------|-------|
| ATOM | 4578 | O | ALA B 197 | 53.910 | -2.609 | 94.549 | 1.00 | 17.67 |
| ATOM | 4579 | N | PHE B 198 | 53.278 | -0.541 | 93.932 | 1.00 | 26.40 |
| ATOM | 4580 | CA | PHE B 198 | 51.956 | -0.950 | 93.495 | 1.00 | 28.19 |
| ATOM | 4581 | CB | PHE B 198 | 51.152 | 0.263 | 93.035 | 1.00 | 29.51 |
| ATOM | 4582 | CG | PHE B 198 | 49.721 | -0.050 | 92.711 | 1.00 | 29.50 |
| ATOM | 4583 | CD1 | PHE B 198 | 48.732 | 0.100 | 93.674 | 1.00 | 32.77 |
| ATOM | 4584 | CD2 | PHE B 198 | 49.367 | -0.533 | 91.455 | 1.00 | 25.82 |
| ATOM | 4585 | CE1 | PHE B 198 | 47.410 | -0.223 | 93.394 | 1.00 | 36.70 |
| ATOM | 4586 | CE2 | PHE B 198 | 48.050 | -0.858 | 91.170 | 1.00 | 29.29 |
| ATOM | 4587 | CZ | PHE B 198 | 47.071 | -0.703 | 92.141 | 1.00 | 33.05 |
| ATOM | 4588 | C | PHE B 198 | 52.170 | -1.858 | 92.284 | 1.00 | 28.28 |
| ATOM | 4589 | O | PHE B 198 | 53.045 | -1.602 | 91.456 | 1.00 | 27.15 |
| ATOM | 4590 | N | PRO B 199 | 51.407 | -2.952 | 92.185 | 1.00 | 31.37 |
| ATOM | 4591 | CD | PRO B 199 | 51.440 | -3.687 | 91.045 | 1.00 | 37.07 |
| ATOM | 4592 | CA | PRO B 199 | 50.386 | -3.369 | 93.144 | 1.00 | 35.32 |
| ATOM | 4593 | CB | PRO B 199 | 49.545 | -4.328 | 92.321 | 1.00 | 33.88 |
| ATOM | 4594 | CG | PRO B 199 | 50.641 | -5.068 | 91.578 | 1.00 | 36.75 |
| ATOM | 4595 | C | PRO B 199 | 51.241 | -4.082 | 94.184 | 1.00 | 36.93 |
| ATOM | 4596 | O | PRO B 199 | 52.308 | -4.603 | 93.860 | 1.00 | 50.93 |
| ATOM | 4597 | N | PHE B 200 | 50.804 | -4.127 | 95.422 | 1.00 | 37.04 |
| ATOM | 4598 | CA | PHE B 200 | 51.644 | -4.763 | 96.421 | 1.00 | 30.13 |
| ATOM | 4599 | CB | PHE B 200 | 51.547 | -3.968 | 97.723 | 1.00 | 28.70 |
| ATOM | 4600 | CG | PHE B 200 | 51.760 | -2.485 | 97.543 | 1.00 | 29.98 |
| ATOM | 4601 | CD1 | PHE B 200 | 50.717 | -1.660 | 97.137 | 1.00 | 28.92 |
| ATOM | 4602 | CD2 | PHE B 200 | 53.016 | -1.919 | 97.746 | 1.00 | 23.60 |
| ATOM | 4603 | CE1 | PHE B 200 | 50.922 | -0.289 | 96.938 | 1.00 | 27.63 |
| ATOM | 4604 | CE2 | PHE B 200 | 53.229 | -0.558 | 97.547 | 1.00 | 23.56 |
| ATOM | 4605 | CZ | PHE B 200 | 52.182 | 0.260 | 97.143 | 1.00 | 28.37 |
| ATOM | 4606 | C | PHE B 200 | 51.296 | -6.227 | 96.658 | 1.00 | 25.51 |
| ATOM | 4607 | O | PHE B 200 | 52.112 | -6.984 | 97.167 | 1.00 | 20.92 |
| ATOM | 4608 | N | GLU B 201 | 50.094 | -6.618 | 96.252 | 1.00 | 27.41 |
| ATOM | 4609 | CA | GLU B 201 | 49.576 | -7.972 | 96.454 | 1.00 | 31.98 |
| ATOM | 4610 | CB | GLU B 201 | 48.056 | -7.928 | 96.487 | 1.00 | 31.57 |
| ATOM | 4611 | CG | GLU B 201 | 47.486 | -6.935 | 97.449 | 1.00 | 39.17 |
| ATOM | 4612 | CD | GLU B 201 | 45.987 | -6.853 | 97.316 | 1.00 | 40.31 |
| ATOM | 4613 | OE1 | GLU B 201 | 45.332 | -7.902 | 97.500 | 1.00 | 38.90 |
| ATOM | 4614 | OE2 | GLU B 201 | 45.475 | -5.751 | 97.019 | 1.00 | 35.04 |
| ATOM | 4615 | C | GLU B 201 | 49.979 | -9.018 | 95.422 | 1.00 | 30.83 |
| ATOM | 4616 | O | GLU B 201 | 49.901 | -10.219 | 95.690 | 1.00 | 26.34 |
| ATOM | 4617 | N | LYS B 202 | 50.362 | -8.573 | 94.234 | 1.00 | 24.95 |
| ATOM | 4618 | CA | LYS B 202 | 50.764 | -9.501 | 93.195 | 1.00 | 22.79 |
| ATOM | 4619 | CB | LYS B 202 | 49.588 | -9.773 | 92.258 | 1.00 | 25.12 |
| ATOM | 4620 | CG | LYS B 202 | 48.484 | -10.523 | 93.000 | 1.00 | 35.38 |
| ATOM | 4621 | CD | LYS B 202 | 47.431 | -11.099 | 92.103 | 1.00 | 38.67 |
| ATOM | 4622 | CE | LYS B 202 | 46.498 | -11.998 | 92.903 | 1.00 | 40.98 |
| ATOM | 4623 | NZ | LYS B 202 | 45.491 | -12.659 | 92.028 | 1.00 | 46.65 |
| ATOM | 4624 | C | LYS B 202 | 51.975 | -9.007 | 92.435 | 1.00 | 24.62 |
| ATOM | 4625 | O | LYS B 202 | 52.355 | -7.838 | 92.549 | 1.00 | 21.83 |
| ATOM | 4626 | N | GLY B 203 | 52.598 | -9.910 | 91.684 | 1.00 | 17.60 |
| ATOM | 4627 | CA | GLY B 203 | 53.779 | -9.545 | 90.928 | 1.00 | 19.41 |
| ATOM | 4628 | C | GLY B 203 | 55.014 | -10.297 | 91.396 | 1.00 | 20.36 |
| ATOM | 4629 | O | GLY B 203 | 56.101 | -10.070 | 90.888 | 1.00 | 23.83 |
| ATOM | 4630 | N | PHE B 204 | 54.855 | -11.201 | 92.358 | 1.00 | 24.82 |
| ATOM | 4631 | CA | PHE B 204 | 55.992 | -11.957 | 92.859 | 1.00 | 24.24 |
| ATOM | 4632 | CB | PHE B 204 | 55.690 | -12.567 | 94.236 | 1.00 | 22.72 |
| ATOM | 4633 | CG | PHE B 204 | 55.485 | -11.549 | 95.322 | 1.00 | 25.26 |
| ATOM | 4634 | CD1 | PHE B 204 | 54.235 | -10.977 | 95.535 | 1.00 | 23.80 |
| ATOM | 4635 | CD2 | PHE B 204 | 56.551 | -11.159 | 96.133 | 1.00 | 20.25 |
| ATOM | 4636 | CE1 | PHE B 204 | 54.048 | -10.036 | 96.545 | 1.00 | 29.98 |
| ATOM | 4637 | CE2 | PHE B 204 | 56.377 | -10.221 | 97.141 | 1.00 | 24.40 |
| ATOM | 4638 | CZ | PHE B 204 | 55.124 | -9.658 | 97.350 | 1.00 | 25.54 |
| ATOM | 4639 | C | PHE B 204 | 56.412 | -13.057 | 91.894 | 1.00 | 25.86 |
| ATOM | 4640 | O | PHE B 204 | 55.613 | -13.540 | 91.091 | 1.00 | 20.65 |
| ATOM | 4641 | N | LEU B 205 | 57.676 | -13.449 | 91.986 | 1.00 | 24.25 |
| ATOM | 4642 | CA | LEU B 205 | 58.233 | -14.472 | 91.114 | 1.00 | 30.66 |
| ATOM | 4643 | CB | LEU B 205 | 59.723 | -14.637 | 91.413 | 1.00 | 34.01 |

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Figure 18-71

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4644 | CG | LEU | B | 205 | 60.495 | -15.669 | 90.592 | 1.00 | 34.12 |
| ATOM | 4645 | CD1 | LEU | B | 205 | 60.356 | -15.382 | 89.109 | 1.00 | 32.95 |
| ATOM | 4646 | CD2 | LEU | B | 205 | 61.957 | -15.629 | 91.005 | 1.00 | 36.49 |
| ATOM | 4647 | C | LEU | B | 205 | 57.535 | -15.827 | 91.205 | 1.00 | 30.51 |
| ATOM | 4648 | O | LEU | B | 205 | 57.467 | -16.562 | 90.220 | 1.00 | 25.89 |
| ATOM | 4649 | N | GLU | B | 206 | 57.010 | -16.147 | 92.382 | 1.00 | 30.43 |
| ATOM | 4650 | CA | GLU | B | 206 | 56.338 | -17.423 | 92.605 | 1.00 | 30.64 |
| ATOM | 4651 | CB | GLU | B | 206 | 56.025 | -17.601 | 94.093 | 1.00 | 34.77 |
| ATOM | 4652 | CG | GLU | B | 206 | 57.227 | -17.512 | 95.033 | 1.00 | 42.50 |
| ATOM | 4653 | CD | GLU | B | 206 | 57.718 | -16.084 | 95.270 | 1.00 | 45.76 |
| ATOM | 4654 | OE1 | GLU | B | 206 | 58.228 | -15.438 | 94.333 | 1.00 | 42.62 |
| ATOM | 4655 | OE2 | GLU | B | 206 | 57.585 | -15.602 | 96.413 | 1.00 | 50.22 |
| ATOM | 4656 | C | GLU | B | 206 | 55.045 | -17.587 | 91.811 | 1.00 | 31.13 |
| ATOM | 4657 | O | GLU | B | 206 | 54.607 | -18.708 | 91.563 | 1.00 | 28.18 |
| ATOM | 4658 | N | GLU | B | 207 | 54.430 | -16.472 | 91.425 | 1.00 | 25.16 |
| ATOM | 4659 | CA | GLU | B | 207 | 53.178 | -16.499 | 90.664 | 1.00 | 28.78 |
| ATOM | 4660 | CB | GLU | B | 207 | 52.546 | -15.107 | 90.695 | 1.00 | 30.76 |
| ATOM | 4661 | CG | GLU | B | 207 | 52.121 | -14.659 | 92.093 | 1.00 | 29.39 |
| ATOM | 4662 | CD | GLU | B | 207 | 52.057 | -13.151 | 92.230 | 1.00 | 27.87 |
| ATOM | 4663 | OE1 | GLU | B | 207 | 51.656 | -12.477 | 91.261 | 1.00 | 24.38 |
| ATOM | 4664 | OE2 | GLU | B | 207 | 52.389 | -12.636 | 93.316 | 1.00 | 25.36 |
| ATOM | 4665 | C | GLU | B | 207 | 53.453 | -16.922 | 89.224 | 1.00 | 29.48 |
| ATOM | 4666 | O | GLU | B | 207 | 53.658 | -16.077 | 88.351 | 1.00 | 27.48 |
| ATOM | 4667 | N | ILE | B | 208 | 53.442 | -18.230 | 88.976 | 1.00 | 26.67 |
| ATOM | 4668 | CA | ILE | B | 208 | 53.735 | -18.754 | 87.646 | 1.00 | 32.60 |
| ATOM | 4669 | CB | ILE | B | 208 | 54.789 | -19.877 | 87.740 | 1.00 | 34.26 |
| ATOM | 4670 | CG2 | ILE | B | 208 | 55.239 | -20.296 | 86.352 | 1.00 | 41.65 |
| ATOM | 4671 | CG1 | ILE | B | 208 | 56.008 | -19.404 | 88.532 | 1.00 | 36.07 |
| ATOM | 4672 | CD1 | ILE | B | 208 | 56.814 | -18.338 | 87.851 | 1.00 | 45.18 |
| ATOM | 4673 | C | ILE | B | 208 | 52.522 | -19.289 | 86.870 | 1.00 | 32.26 |
| ATOM | 4674 | O | ILE | B | 208 | 52.668 | -19.799 | 85.759 | 1.00 | 27.43 |
| ATOM | 4675 | N | GLY | B | 209 | 51.328 | -19.165 | 87.442 | 1.00 | 32.60 |
| ATOM | 4676 | CA | GLY | B | 209 | 50.139 | -19.652 | 86.760 | 1.00 | 35.07 |
| ATOM | 4677 | C | GLY | B | 209 | 49.565 | -20.892 | 87.420 | 1.00 | 36.19 |
| ATOM | 4678 | O | GLY | B | 209 | 50.230 | -21.524 | 88.235 | 1.00 | 31.61 |
| ATOM | 4679 | N | GLU | B | 210 | 48.335 | -21.245 | 87.066 | 1.00 | 36.98 |
| ATOM | 4680 | CA | GLU | B | 210 | 47.677 | -22.412 | 87.647 | 1.00 | 40.60 |
| ATOM | 4681 | CB | GLU | B | 210 | 46.633 | -21.964 | 88.672 | 1.00 | 37.98 |
| ATOM | 4682 | CG | GLU | B | 210 | 45.446 | -21.234 | 88.058 | 1.00 | 42.78 |
| ATOM | 4683 | CD | GLU | B | 210 | 44.470 | -20.717 | 89.098 | 1.00 | 48.41 |
| ATOM | 4684 | OE1 | GLU | B | 210 | 43.400 | -20.202 | 88.709 | 1.00 | 51.03 |
| ATOM | 4685 | OE2 | GLU | B | 210 | 44.778 | -20.814 | 90.306 | 1.00 | 49.90 |
| ATOM | 4686 | C | GLU | B | 210 | 46.996 | -23.248 | 86.564 | 1.00 | 39.48 |
| ATOM | 4687 | O | GLU | B | 210 | 46.709 | -22.751 | 85.471 | 1.00 | 33.65 |
| ATOM | 4688 | N | GLY | B | 211 | 46.736 | -24.515 | 86.876 | 1.00 | 39.18 |
| ATOM | 4689 | CA | GLY | B | 211 | 46.087 | -25.399 | 85.923 | 1.00 | 38.43 |
| ATOM | 4690 | C | GLY | B | 211 | 46.877 | -25.500 | 84.637 | 1.00 | 40.29 |
| ATOM | 4691 | O | GLY | B | 211 | 48.101 | -25.610 | 84.666 | 1.00 | 39.39 |
| ATOM | 4692 | N | LYS | B | 212 | 46.187 | -25.458 | 83.504 | 1.00 | 40.90 |
| ATOM | 4693 | CA | LYS | B | 212 | 46.864 | -25.538 | 82.219 | 1.00 | 43.53 |
| ATOM | 4694 | CB | LYS | B | 212 | 45.842 | -25.548 | 81.080 | 1.00 | 47.87 |
| ATOM | 4695 | CG | LYS | B | 212 | 44.795 | -26.665 | 81.144 | 1.00 | 53.09 |
| ATOM | 4696 | CD | LYS | B | 212 | 45.398 | -28.076 | 81.130 | 1.00 | 58.61 |
| ATOM | 4697 | CE | LYS | B | 212 | 46.069 | -28.454 | 82.452 | 1.00 | 59.78 |
| ATOM | 4698 | NZ | LYS | B | 212 | 46.670 | -29.825 | 82.420 | 1.00 | 62.17 |
| ATOM | 4699 | C | LYS | B | 212 | 47.823 | -24.363 | 82.040 | 1.00 | 38.84 |
| ATOM | 4700 | O | LYS | B | 212 | 48.797 | -24.457 | 81.295 | 1.00 | 40.33 |
| ATOM | 4701 | N | GLY | B | 213 | 47.543 | -23.262 | 82.731 | 1.00 | 37.20 |
| ATOM | 4702 | CA | GLY | B | 213 | 48.384 | -22.081 | 82.627 | 1.00 | 34.66 |
| ATOM | 4703 | C | GLY | B | 213 | 49.625 | -22.107 | 83.505 | 1.00 | 37.09 |
| ATOM | 4704 | O | GLY | B | 213 | 50.425 | -21.165 | 83.489 | 1.00 | 25.85 |
| ATOM | 4705 | N | LYS | B | 214 | 49.794 | -23.180 | 84.273 | 1.00 | 33.33 |
| ATOM | 4706 | CA | LYS | B | 214 | 50.953 | -23.297 | 85.148 | 1.00 | 37.90 |
| ATOM | 4707 | CB | LYS | B | 214 | 50.886 | -24.598 | 85.954 | 1.00 | 38.89 |
| ATOM | 4708 | CG | LYS | B | 214 | 52.032 | -24.786 | 86.938 | 1.00 | 39.29 |
| ATOM | 4709 | CD | LYS | B | 214 | 51.876 | -26.094 | 87.704 | 1.00 | 43.60 |

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Figure 18-72

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4710 | CE | LYS | B | 214 | 53.047 | -26.334 | 88.640 | 1.00 | 47.36 |
| ATOM | 4711 | NZ | LYS | B | 214 | 53.165 | -25.264 | 89.666 | 1.00 | 54.03 |
| ATOM | 4712 | C | LYS | B | 214 | 52.209 | -23.275 | 84.291 | 1.00 | 34.16 |
| ATOM | 4713 | O | LYS | B | 214 | 52.404 | -24.136 | 83.438 | 1.00 | 34.70 |
| ATOM | 4714 | N | GLY | B | 215 | 53.057 | -22.279 | 84.523 | 1.00 | 33.58 |
| ATOM | 4715 | CA | GLY | B | 215 | 54.275 | -22.152 | 83.743 | 1.00 | 28.27 |
| ATOM | 4716 | C | GLY | B | 215 | 54.104 | -21.155 | 82.605 | 1.00 | 31.02 |
| ATOM | 4717 | O | GLY | B | 215 | 55.033 | -20.911 | 81.833 | 1.00 | 23.68 |
| ATOM | 4718 | N | TYR | B | 216 | 52.918 | -20.564 | 82.493 | 1.00 | 22.45 |
| ATOM | 4719 | CA | TYR | B | 216 | 52.683 | -19.605 | 81.426 | 1.00 | 24.03 |
| ATOM | 4720 | CB | TYR | B | 216 | 51.458 | -20.013 | 80.603 | 1.00 | 17.60 |
| ATOM | 4721 | CG | TYR | B | 216 | 51.682 | -21.291 | 79.806 | 1.00 | 25.96 |
| ATOM | 4722 | CD1 | TYR | B | 216 | 51.692 | -22.538 | 80.435 | 1.00 | 21.41 |
| ATOM | 4723 | CE1 | TYR | B | 216 | 51.988 | -23.704 | 79.729 | 1.00 | 23.78 |
| ATOM | 4724 | CD2 | TYR | B | 216 | 51.970 | -21.242 | 78.439 | 1.00 | 19.62 |
| ATOM | 4725 | CE2 | TYR | B | 216 | 52.269 | -22.402 | 77.722 | 1.00 | 26.39 |
| ATOM | 4726 | CZ | TYR | B | 216 | 52.277 | -23.630 | 78.379 | 1.00 | 29.35 |
| ATOM | 4727 | OH | TYR | B | 216 | 52.577 | -24.782 | 77.690 | 1.00 | 27.75 |
| ATOM | 4728 | C | TYR | B | 216 | 52.575 | -18.153 | 81.884 | 1.00 | 24.53 |
| ATOM | 4729 | O | TYR | B | 216 | 52.065 | -17.298 | 81.159 | 1.00 | 18.99 |
| ATOM | 4730 | N | ASN | B | 217 | 53.052 | -17.886 | 83.098 | 1.00 | 21.41 |
| ATOM | 4731 | CA | ASN | B | 217 | 53.073 | -16.534 | 83.642 | 1.00 | 21.23 |
| ATOM | 4732 | CB | ASN | B | 217 | 51.954 | -16.325 | 84.669 | 1.00 | 16.78 |
| ATOM | 4733 | CG | ASN | B | 217 | 51.882 | -14.889 | 85.162 | 1.00 | 22.07 |
| ATOM | 4734 | OD1 | ASN | B | 217 | 52.506 | -14.521 | 86.163 | 1.00 | 23.13 |
| ATOM | 4735 | ND2 | ASN | B | 217 | 51.146 | -14.058 | 84.435 | 1.00 | 19.26 |
| ATOM | 4736 | C | ASN | B | 217 | 54.437 | -16.339 | 84.291 | 1.00 | 19.40 |
| ATOM | 4737 | O | ASN | B | 217 | 54.857 | -17.145 | 85.124 | 1.00 | 19.28 |
| ATOM | 4738 | N | LEU | B | 218 | 55.130 | -15.273 | 83.905 | 1.00 | 18.65 |
| ATOM | 4739 | CA | LEU | B | 218 | 56.459 | -15.004 | 84.444 | 1.00 | 16.41 |
| ATOM | 4740 | CB | LEU | B | 218 | 57.512 | -15.244 | 83.368 | 1.00 | 18.29 |
| ATOM | 4741 | CG | LEU | B | 218 | 58.851 | -15.872 | 83.782 | 1.00 | 28.15 |
| ATOM | 4742 | CD1 | LEU | B | 218 | 59.873 | -15.563 | 82.695 | 1.00 | 20.50 |
| ATOM | 4743 | CD2 | LEU | B | 218 | 59.332 | -15.348 | 85.116 | 1.00 | 22.53 |
| ATOM | 4744 | C | LEU | B | 218 | 56.595 | -13.562 | 84.926 | 1.00 | 17.89 |
| ATOM | 4745 | O | LEU | B | 218 | 56.469 | -12.627 | 84.128 | 1.00 | 14.48 |
| ATOM | 4746 | N | ASN | B | 219 | 56.859 | -13.395 | 86.219 | 1.00 | 14.09 |
| ATOM | 4747 | CA | ASN | B | 219 | 57.044 | -12.075 | 86.821 | 1.00 | 18.41 |
| ATOM | 4748 | CB | ASN | B | 219 | 56.238 | -11.922 | 88.111 | 1.00 | 14.64 |
| ATOM | 4749 | CG | ASN | B | 219 | 54.748 | -11.898 | 87.868 | 1.00 | 27.12 |
| ATOM | 4750 | OD1 | ASN | B | 219 | 54.286 | -11.332 | 86.880 | 1.00 | 20.21 |
| ATOM | 4751 | ND2 | ASN | B | 219 | 53.982 | -12.480 | 88.787 | 1.00 | 23.62 |
| ATOM | 4752 | C | ASN | B | 219 | 58.504 | -11.843 | 87.172 | 1.00 | 20.39 |
| ATOM | 4753 | O | ASN | B | 219 | 59.115 | -12.672 | 87.841 | 1.00 | 20.41 |
| ATOM | 4754 | N | ILE | B | 220 | 59.056 | -10.717 | 86.729 | 1.00 | 15.11 |
| ATOM | 4755 | CA | ILE | B | 220 | 60.441 | -10.394 | 87.033 | 1.00 | 17.16 |
| ATOM | 4756 | CB | ILE | B | 220 | 61.250 | -10.083 | 85.740 | 1.00 | 20.78 |
| ATOM | 4757 | CG2 | ILE | B | 220 | 62.736 | -9.821 | 86.094 | 1.00 | 18.08 |
| ATOM | 4758 | CG1 | ILE | B | 220 | 61.138 | -11.250 | 84.748 | 1.00 | 17.62 |
| ATOM | 4759 | CD1 | ILE | B | 220 | 61.646 | -12.590 | 85.273 | 1.00 | 20.72 |
| ATOM | 4760 | C | ILE | B | 220 | 60.475 | -9.161 | 87.947 | 1.00 | 21.17 |
| ATOM | 4761 | O | ILE | B | 220 | 60.565 | -8.036 | 87.470 | 1.00 | 16.03 |
| ATOM | 4762 | N | PRO | B | 221 | 60.367 | -9.357 | 89.274 | 1.00 | 21.74 |
| ATOM | 4763 | CD | PRO | B | 221 | 60.135 | -10.619 | 90.000 | 1.00 | 22.96 |
| ATOM | 4764 | CA | PRO | B | 221 | 60.394 | -8.225 | 90.213 | 1.00 | 19.16 |
| ATOM | 4765 | CB | PRO | B | 221 | 59.947 | -8.869 | 91.523 | 1.00 | 19.40 |
| ATOM | 4766 | CG | PRO | B | 221 | 60.564 | -10.251 | 91.407 | 1.00 | 23.02 |
| ATOM | 4767 | C | PRO | B | 221 | 61.799 | -7.634 | 90.289 | 1.00 | 22.42 |
| ATOM | 4768 | O | PRO | B | 221 | 62.780 | -8.369 | 90.425 | 1.00 | 20.71 |
| ATOM | 4769 | N | LEU | B | 222 | 61.899 | -6.309 | 90.202 | 1.00 | 22.74 |
| ATOM | 4770 | CA | LEU | B | 222 | 63.198 | -5.643 | 90.223 | 1.00 | 21.18 |
| ATOM | 4771 | CB | LEU | B | 222 | 63.453 | -4.993 | 88.850 | 1.00 | 17.21 |
| ATOM | 4772 | CG | LEU | B | 222 | 63.467 | -6.027 | 87.721 | 1.00 | 20.26 |
| ATOM | 4773 | CD1 | LEU | B | 222 | 63.453 | -5.354 | 86.361 | 1.00 | 20.00 |
| ATOM | 4774 | CD2 | LEU | B | 222 | 64.696 | -6.908 | 87.881 | 1.00 | 21.93 |
| ATOM | 4775 | C | LEU | B | 222 | 63.335 | -4.616 | 91.353 | 1.00 | 20.04 |

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Figure 18-73

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4776 | O | LEU | B | 222 | 62.350 | -4.030 | 91.806 | 1.00 | 17.58 |
| ATOM | 4777 | N | PRO | B | 223 | 64.571 | -4.394 | 91.830 | 1.00 | 19.48 |
| ATOM | 4778 | CD | PRO | B | 223 | 65.806 | -5.072 | 91.400 | 1.00 | 16.80 |
| ATOM | 4779 | CA | PRO | B | 223 | 64.873 | -3.454 | 92.915 | 1.00 | 20.38 |
| ATOM | 4780 | CB | PRO | B | 223 | 66.274 | -3.881 | 93.327 | 1.00 | 26.11 |
| ATOM | 4781 | CG | PRO | B | 223 | 66.884 | -4.161 | 91.973 | 1.00 | 19.74 |
| ATOM | 4782 | C | PRO | B | 223 | 64.818 | -1.971 | 92.553 | 1.00 | 21.39 |
| ATOM | 4783 | O | PRO | B | 223 | 64.815 | -1.598 | 91.380 | 1.00 | 17.16 |
| ATOM | 4784 | N | LYS | B | 224 | 64.798 | -1.142 | 93.589 | 1.00 | 20.65 |
| ATOM | 4785 | CA | LYS | B | 224 | 64.755 | 0.311 | 93.462 | 1.00 | 27.00 |
| ATOM | 4786 | CB | LYS | B | 224 | 64.577 | 0.938 | 94.844 | 1.00 | 36.47 |
| ATOM | 4787 | CG | LYS | B | 224 | 63.415 | 0.389 | 95.651 | 1.00 | 37.72 |
| ATOM | 4788 | CD | LYS | B | 224 | 63.541 | 0.833 | 97.101 | 1.00 | 42.06 |
| ATOM | 4789 | CE | LYS | B | 224 | 62.420 | 0.276 | 97.955 | 1.00 | 45.18 |
| ATOM | 4790 | NZ | LYS | B | 224 | 62.645 | 0.570 | 99.399 | 1.00 | 46.30 |
| ATOM | 4791 | C | LYS | B | 224 | 66.071 | 0.808 | 92.874 | 1.00 | 27.01 |
| ATOM | 4792 | O | LYS | B | 224 | 67.098 | 0.139 | 92.995 | 1.00 | 21.54 |
| ATOM | 4793 | N | GLY | B | 225 | 66.038 | 1.989 | 92.259 | 1.00 | 22.66 |
| ATOM | 4794 | CA | GLY | B | 225 | 67.239 | 2.565 | 91.669 | 1.00 | 25.67 |
| ATOM | 4795 | C | GLY | B | 225 | 67.768 | 1.809 | 90.459 | 1.00 | 24.95 |
| ATOM | 4796 | O | GLY | B | 225 | 68.917 | 1.975 | 90.069 | 1.00 | 26.83 |
| ATOM | 4797 | N | LEU | B | 226 | 66.926 | 0.980 | 89.855 | 1.00 | 21.79 |
| ATOM | 4798 | CA | LEU | B | 226 | 67.319 | 0.180 | 88.692 | 1.00 | 22.91 |
| ATOM | 4799 | CB | LEU | B | 226 | 66.067 | -0.473 | 88.099 | 1.00 | 23.29 |
| ATOM | 4800 | CG | LEU | B | 226 | 66.238 | -1.605 | 87.091 | 1.00 | 26.71 |
| ATOM | 4801 | CD1 | LEU | B | 226 | 66.846 | -2.804 | 87.813 | 1.00 | 26.44 |
| ATOM | 4802 | CD2 | LEU | B | 226 | 64.877 | -1.997 | 86.508 | 1.00 | 22.96 |
| ATOM | 4803 | C | LEU | B | 226 | 68.008 | 1.017 | 87.603 | 1.00 | 22.66 |
| ATOM | 4804 | O | LEU | B | 226 | 67.517 | 2.087 | 87.250 | 1.00 | 20.19 |
| ATOM | 4805 | N | ASN | B | 227 | 69.134 | 0.549 | 87.060 | 1.00 | 15.52 |
| ATOM | 4806 | CA | ASN | B | 227 | 69.794 | 1.317 | 85.998 | 1.00 | 19.49 |
| ATOM | 4807 | CB | ASN | B | 227 | 71.304 | 1.474 | 86.270 | 1.00 | 20.43 |
| ATOM | 4808 | CG | ASN | B | 227 | 72.062 | 0.161 | 86.206 | 1.00 | 28.97 |
| ATOM | 4809 | OD1 | ASN | B | 227 | 72.015 | -0.546 | 85.199 | 1.00 | 24.30 |
| ATOM | 4810 | ND2 | ASN | B | 227 | 72.786 | -0.160 | 87.276 | 1.00 | 20.88 |
| ATOM | 4811 | C | ASN | B | 227 | 69.548 | 0.671 | 84.630 | 1.00 | 21.26 |
| ATOM | 4812 | O | ASN | B | 227 | 69.004 | -0.432 | 84.555 | 1.00 | 18.90 |
| ATOM | 4813 | N | ASP | B | 228 | 69.949 | 1.347 | 83.552 | 1.00 | 20.98 |
| ATOM | 4814 | CA | ASP | B | 228 | 69.720 | 0.817 | 82.208 | 1.00 | 22.61 |
| ATOM | 4815 | CB | ASP | B | 228 | 70.270 | 1.753 | 31.126 | 1.00 | 23.46 |
| ATOM | 4816 | CG | ASP | B | 228 | 69.596 | 3.113 | 81.119 | 1.00 | 26.12 |
| ATOM | 4817 | OD1 | ASP | B | 228 | 68.387 | 3.193 | 81.415 | 1.00 | 26.75 |
| ATOM | 4818 | OD2 | ASP | B | 228 | 70.276 | 4.101 | 80.773 | 1.00 | 30.22 |
| ATOM | 4819 | C | ASP | B | 228 | 70.286 | -0.573 | 81.952 | 1.00 | 23.49 |
| ATOM | 4820 | O | ASP | B | 228 | 69.651 | -1.390 | 81.288 | 1.00 | 19.31 |
| ATOM | 4821 | N | ASN | B | 229 | 71.484 | -0.836 | 82.453 | 1.00 | 22.24 |
| ATOM | 4822 | CA | ASN | B | 229 | 72.111 | -2.135 | 82.250 | 1.00 | 23.30 |
| ATOM | 4823 | CB | ASN | B | 229 | 73.562 | -2.101 | 82.737 | 1.00 | 20.99 |
| ATOM | 4824 | CG | ASN | B | 229 | 74.441 | -1.237 | 81.859 | 1.00 | 25.71 |
| ATOM | 4825 | OD1 | ASN | B | 229 | 74.644 | -1.538 | 80.678 | 1.00 | 26.40 |
| ATOM | 4826 | ND2 | ASN | B | 229 | 74.955 | -0.151 | 82.417 | 1.00 | 27.44 |
| ATOM | 4827 | C | ASN | B | 229 | 71.341 | -3.252 | 82.943 | 1.00 | 23.74 |
| ATOM | 4828 | O | ASN | B | 229 | 71.207 | -4.346 | 82.402 | 1.00 | 20.51 |
| ATOM | 4829 | N | GLU | B | 230 | 70.832 | -2.976 | 84.139 | 1.00 | 23.06 |
| ATOM | 4830 | CA | GLU | B | 230 | 70.069 | -3.977 | 84.874 | 1.00 | 23.01 |
| ATOM | 4831 | CB | GLU | B | 230 | 69.799 | -3.480 | 86.297 | 1.00 | 24.73 |
| ATOM | 4832 | CG | GLU | B | 230 | 71.069 | -3.201 | 87.087 | 1.00 | 27.28 |
| ATOM | 4833 | CD | GLU | B | 230 | 70.792 | -2.649 | 88.470 | 1.00 | 27.47 |
| ATOM | 4834 | OE1 | GLU | B | 230 | 70.086 | -1.625 | 88.569 | 1.00 | 27.87 |
| ATOM | 4835 | OE2 | GLU | B | 230 | 71.286 | -3.232 | 89.455 | 1.00 | 26.79 |
| ATOM | 4836 | C | GLU | B | 230 | 68.749 | -4.281 | 84.146 | 1.00 | 24.25 |
| ATOM | 4837 | O | GLU | B | 230 | 68.347 | -5.445 | 84.022 | 1.00 | 15.89 |
| ATOM | 4838 | N | PHE | B | 231 | 68.091 | -3.242 | 83.637 | 1.00 | 21.46 |
| ATOM | 4839 | CA | PHE | B | 231 | 66.814 | -3.429 | 82.933 | 1.00 | 22.84 |
| ATOM | 4840 | CB | PHE | B | 231 | 66.210 | -2.079 | 82.529 | 1.00 | 23.96 |
| ATOM | 4841 | CG | PHE | B | 231 | 64.803 | -2.182 | 81.975 | 1.00 | 26.13 |

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Figure 18-74

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4842 | CD1 | PHE | B | 231 | 63.738 | -2.514 | 82.805 | 1.00 | 25.00 |
| ATOM | 4843 | CD2 | PHE | B | 231 | 64.550 | -1.956 | 80.627 | 1.00 | 22.93 |
| ATOM | 4844 | CE1 | PHE | B | 231 | 62.440 | -2.618 | 82.304 | 1.00 | 25.03 |
| ATOM | 4845 | CE2 | PHE | B | 231 | 63.250 | -2.059 | 80.114 | 1.00 | 27.46 |
| ATOM | 4846 | CZ | PHE | B | 231 | 62.196 | -2.390 | 80.957 | 1.00 | 20.25 |
| ATOM | 4847 | C | PHE | B | 231 | 66.978 | -4.288 | 81.677 | 1.00 | 23.14 |
| ATOM | 4848 | O | PHE | B | 231 | 66.221 | -5.239 | 81.464 | 1.00 | 20.02 |
| ATOM | 4849 | N | LEU | B | 232 | 67.963 | -3.952 | 80.845 | 1.00 | 22.02 |
| ATOM | 4850 | CA | LEU | B | 232 | 68.200 | -4.697 | 79.614 | 1.00 | 19.97 |
| ATOM | 4851 | CB | LEU | B | 232 | 69.192 | -3.942 | 78.734 | 1.00 | 24.99 |
| ATOM | 4852 | CG | LEU | B | 232 | 68.665 | -2.581 | 78.263 | 1.00 | 29.73 |
| ATOM | 4853 | CD1 | LEU | B | 232 | 69.746 | -1.856 | 77.454 | 1.00 | 28.11 |
| ATOM | 4854 | CD2 | LEU | B | 232 | 67.409 | -2.784 | 77.414 | 1.00 | 26.54 |
| ATOM | 4855 | C | LEU | B | 232 | 68.688 | -6.119 | 79.898 | 1.00 | 19.25 |
| ATOM | 4856 | O | LEU | B | 232 | 68.365 | -7.051 | 79.162 | 1.00 | 19.49 |
| ATOM | 4857 | N | PHE | B | 233 | 69.468 | -6.280 | 80.962 | 1.00 | 20.50 |
| ATOM | 4858 | CA | PHE | B | 233 | 69.950 | -7.599 | 81.378 | 1.00 | 20.70 |
| ATOM | 4859 | CB | PHE | B | 233 | 70.825 | -7.471 | 82.632 | 1.00 | 23.75 |
| ATOM | 4860 | CG | PHE | B | 233 | 71.217 | -8.790 | 83.239 | 1.00 | 28.58 |
| ATOM | 4861 | CD1 | PHE | B | 233 | 72.285 | -9.519 | 82.731 | 1.00 | 30.48 |
| ATOM | 4862 | CD2 | PHE | B | 233 | 70.481 | -9.328 | 84.294 | 1.00 | 25.32 |
| ATOM | 4863 | CE1 | PHE | B | 233 | 72.617 | -10.762 | 83.262 | 1.00 | 31.87 |
| ATOM | 4864 | CE2 | PHE | B | 233 | 70.803 | -10.573 | 84.832 | 1.00 | 31.26 |
| ATOM | 4865 | CZ | PHE | B | 233 | 71.871 | -11.292 | 84.317 | 1.00 | 32.29 |
| ATOM | 4866 | C | PHE | B | 233 | 68.712 | -8.439 | 81.727 | 1.00 | 20.23 |
| ATOM | 4867 | O | PHE | B | 233 | 68.553 | -9.567 | 81.270 | 1.00 | 21.56 |
| ATOM | 4868 | N | ALA | B | 234 | 67.842 | -7.878 | 82.560 | 1.00 | 21.26 |
| ATOM | 4869 | CA | ALA | B | 234 | 66.626 | -8.576 | 82.963 | 1.00 | 19.60 |
| ATOM | 4870 | CB | ALA | B | 234 | 65.835 | -7.733 | 83.950 | 1.00 | 19.25 |
| ATOM | 4871 | C | ALA | B | 234 | 65.772 | -8.898 | 81.749 | 1.00 | 18.87 |
| ATOM | 4872 | O | ALA | B | 234 | 65.253 | -10.010 | 81.624 | 1.00 | 21.91 |
| ATOM | 4873 | N | LEU | B | 235 | 65.634 | -7.934 | 80.845 | 1.00 | 20.29 |
| ATOM | 4874 | CA | LEU | B | 235 | 64.822 | -8.141 | 79.652 | 1.00 | 19.53 |
| ATOM | 4875 | CB | LEU | B | 235 | 64.773 | -6.874 | 78.795 | 1.00 | 24.07 |
| ATOM | 4876 | CG | LEU | B | 235 | 63.465 | -6.607 | 78.024 | 1.00 | 27.87 |
| ATOM | 4877 | CD1 | LEU | B | 235 | 63.783 | -5.813 | 76.770 | 1.00 | 20.77 |
| ATOM | 4878 | CD2 | LEU | B | 235 | 62.761 | -7.897 | 77.664 | 1.00 | 26.94 |
| ATOM | 4879 | C | LEU | B | 235 | 65.376 | -9.276 | 78.795 | 1.00 | 20.79 |
| ATOM | 4880 | O | LEU | B | 235 | 64.648 | -10.205 | 78.431 | 1.00 | 18.25 |
| ATOM | 4881 | N | GLU | B | 236 | 66.665 | -9.191 | 78.462 | 1.00 | 19.33 |
| ATOM | 4882 | CA | GLU | B | 236 | 67.303 | -10.206 | 77.629 | 1.00 | 27.93 |
| ATOM | 4883 | CB | GLU | B | 236 | 68.777 | -9.853 | 77.384 | 1.00 | 31.06 |
| ATOM | 4884 | CG | GLU | B | 236 | 68.969 | -8.597 | 76.548 | 1.00 | 43.60 |
| ATOM | 4885 | CD | GLU | B | 236 | 70.428 | -8.292 | 76.259 | 1.00 | 45.19 |
| ATOM | 4886 | OE1 | GLU | B | 236 | 70.697 | -7.309 | 75.538 | 1.00 | 48.77 |
| ATOM | 4887 | OE2 | GLU | B | 236 | 71.300 | -9.032 | 76.751 | 1.00 | 52.72 |
| ATOM | 4888 | C | GLU | B | 236 | 67.201 | -11.607 | 78.209 | 1.00 | 24.89 |
| ATOM | 4889 | O | GLU | B | 236 | 66.861 | -12.552 | 77.501 | 1.00 | 22.06 |
| ATOM | 4890 | N | LYS | B | 237 | 67.520 | -11.748 | 79.492 | 1.00 | 24.20 |
| ATOM | 4891 | CA | LYS | B | 237 | 67.449 | -13.058 | 80.130 | 1.00 | 27.10 |
| ATOM | 4892 | CB | LYS | B | 237 | 67.989 | -12.984 | 81.562 | 1.00 | 23.43 |
| ATOM | 4893 | CG | LYS | B | 237 | 69.466 | -12.641 | 81.650 | 1.00 | 29.46 |
| ATOM | 4894 | CD | LYS | B | 237 | 70.305 | -13.683 | 80.924 | 1.00 | 31.65 |
| ATOM | 4895 | CE | LYS | B | 237 | 71.782 | -13.356 | 80.993 | 1.00 | 39.70 |
| ATOM | 4896 | NZ | LYS | B | 237 | 72.580 | -14.363 | 80.242 | 1.00 | 46.74 |
| ATOM | 4897 | C | LYS | B | 237 | 66.019 | -13.615 | 80.143 | 1.00 | 30.92 |
| ATOM | 4898 | O | LYS | B | 237 | 65.789 | -14.766 | 79.763 | 1.00 | 31.42 |
| ATOM | 4899 | N | SER | B | 238 | 65.057 | -12.806 | 80.573 | 1.00 | 25.86 |
| ATOM | 4900 | CA | SER | B | 238 | 63.677 | -13.280 | 80.620 | 1.00 | 27.98 |
| ATOM | 4901 | CB | SER | B | 238 | 62.776 | -12.241 | 81.289 | 1.00 | 23.89 |
| ATOM | 4902 | OG | SER | B | 238 | 62.756 | -11.028 | 80.565 | 1.00 | 29.27 |
| ATOM | 4903 | C | SER | B | 238 | 63.145 | -13.642 | 79.229 | 1.00 | 28.32 |
| ATOM | 4904 | O | SER | B | 238 | 62.387 | -14.605 | 79.089 | 1.00 | 29.65 |
| ATOM | 4905 | N | LEU | B | 239 | 63.536 | -12.886 | 78.203 | 1.00 | 27.39 |
| ATOM | 4906 | CA | LEU | B | 239 | 63.079 | -13.192 | 76.846 | 1.00 | 32.52 |
| ATOM | 4907 | CB | LEU | B | 239 | 63.544 | -12.129 | 75.837 | 1.00 | 30.53 |

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Figure 18-75

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4908 | CG | LEU | B | 239 | 62.833 | -10.772 | 75.895 | 1.00 | 36.06 |
| ATOM | 4909 | CD1 | LEU | B | 239 | 63.404 | -9.836 | 74.842 | 1.00 | 29.64 |
| ATOM | 4910 | CD2 | LEU | B | 239 | 61.338 | -10.976 | 75.667 | 1.00 | 30.73 |
| ATOM | 4911 | C | LEU | B | 239 | 63.598 | -14.563 | 76.430 | 1.00 | 34.15 |
| ATOM | 4912 | O | LEU | B | 239 | 62.879 | -15.340 | 75.803 | 1.00 | 33.23 |
| ATOM | 4913 | N | GLU | B | 240 | 64.844 | -14.859 | 76.788 | 1.00 | 31.39 |
| ATOM | 4914 | CA | GLU | B | 240 | 65.434 | -16.152 | 76.472 | 1.00 | 33.79 |
| ATOM | 4915 | CB | GLU | B | 240 | 66.859 | -16.238 | 77.011 | 1.00 | 38.51 |
| ATOM | 4916 | CG | GLU | B | 240 | 67.878 | -15.407 | 76.275 | 1.00 | 40.56 |
| ATOM | 4917 | CD | GLU | B | 240 | 69.256 | -15.532 | 76.903 | 1.00 | 48.20 |
| ATOM | 4918 | OE1 | GLU | B | 240 | 69.685 | -16.679 | 77.161 | 1.00 | 45.36 |
| ATOM | 4919 | OE2 | GLU | B | 240 | 69.912 | -14.492 | 77.130 | 1.00 | 48.21 |
| ATOM | 4920 | C | GLU | B | 240 | 64.604 | -17.258 | 77.108 | 1.00 | 33.23 |
| ATOM | 4921 | O | GLU | B | 240 | 64.391 | -18.310 | 76.510 | 1.00 | 32.15 |
| ATOM | 4922 | N | ILE | B | 241 | 64.146 | -17.017 | 78.331 | 1.00 | 29.72 |
| ATOM | 4923 | CA | ILE | B | 241 | 63.328 | -17.989 | 79.047 | 1.00 | 29.85 |
| ATOM | 4924 | CB | ILE | B | 241 | 63.006 | -17.489 | 80.466 | 1.00 | 30.42 |
| ATOM | 4925 | CG2 | ILE | B | 241 | 62.049 | -18.456 | 81.162 | 1.00 | 29.88 |
| ATOM | 4926 | CG1 | ILE | B | 241 | 64.309 | -17.311 | 81.254 | 1.00 | 29.77 |
| ATOM | 4927 | CD1 | ILE | B | 241 | 64.118 | -16.760 | 82.654 | 1.00 | 32.92 |
| ATOM | 4928 | C | ILE | B | 241 | 62.016 | -18.247 | 78.298 | 1.00 | 34.65 |
| ATOM | 4929 | O | ILE | B | 241 | 61.592 | -19.396 | 78.149 | 1.00 | 30.22 |
| ATOM | 4930 | N | VAL | B | 242 | 61.379 | -17.178 | 77.823 | 1.00 | 31.16 |
| ATOM | 4931 | CA | VAL | B | 242 | 60.114 | -17.312 | 77.105 | 1.00 | 34.55 |
| ATOM | 4932 | CB | VAL | B | 242 | 59.476 | -15.937 | 76.825 | 1.00 | 30.77 |
| ATOM | 4933 | CG1 | VAL | B | 242 | 58.191 | -16.113 | 76.038 | 1.00 | 32.18 |
| ATOM | 4934 | CG2 | VAL | B | 242 | 59.201 | -15.214 | 78.140 | 1.00 | 31.57 |
| ATOM | 4935 | C | VAL | B | 242 | 60.320 | -18.042 | 75.787 | 1.00 | 36.56 |
| ATOM | 4936 | O | VAL | B | 242 | 59.572 | -18.959 | 75.453 | 1.00 | 33.93 |
| ATOM | 4937 | N | LYS | B | 243 | 61.337 | -17.627 | 75.042 | 1.00 | 38.64 |
| ATOM | 4938 | CA | LYS | B | 243 | 61.659 | -18.241 | 73.760 | 1.00 | 44.36 |
| ATOM | 4939 | CB | LYS | B | 243 | 62.966 | -17.659 | 73.214 | 1.00 | 48.33 |
| ATOM | 4940 | CG | LYS | B | 243 | 62.810 | -16.399 | 72.386 | 1.00 | 53.88 |
| ATOM | 4941 | CD | LYS | B | 243 | 62.185 | -16.718 | 71.036 | 1.00 | 53.72 |
| ATOM | 4942 | CE | LYS | B | 243 | 63.056 | -17.681 | 70.242 | 1.00 | 54.69 |
| ATOM | 4943 | NZ | LYS | B | 243 | 62.456 | -18.025 | 68.923 | 1.00 | 57.75 |
| ATOM | 4944 | C | LYS | B | 243 | 61.793 | -19.755 | 73.824 | 1.00 | 43.21 |
| ATOM | 4945 | O | LYS | B | 243 | 61.432 | -20.455 | 72.884 | 1.00 | 42.92 |
| ATOM | 4946 | N | GLU | B | 244 | 62.312 | -20.257 | 74.935 | 1.00 | 45.77 |
| ATOM | 4947 | CA | GLU | B | 244 | 62.528 | -21.687 | 75.085 | 1.00 | 47.72 |
| ATOM | 4948 | CB | GLU | B | 244 | 63.669 | -21.925 | 76.075 | 1.00 | 50.89 |
| ATOM | 4949 | CG | GLU | B | 244 | 64.080 | -23.378 | 76.208 | 1.00 | 57.16 |
| ATOM | 4950 | CD | GLU | B | 244 | 65.223 | -23.564 | 77.173 | 1.00 | 57.74 |
| ATOM | 4951 | OE1 | GLU | B | 244 | 66.295 | -22.967 | 76.942 | 1.00 | 60.18 |
| ATOM | 4952 | OE2 | GLU | B | 244 | 65.049 | -24.308 | 78.160 | 1.00 | 61.59 |
| ATOM | 4953 | C | GLU | B | 244 | 61.312 | -22.507 | 75.505 | 1.00 | 47.78 |
| ATOM | 4954 | O | GLU | B | 244 | 61.376 | -23.736 | 75.544 | 1.00 | 51.39 |
| ATOM | 4955 | N | VAL | B | 245 | 60.200 | -21.851 | 75.805 | 1.00 | 43.31 |
| ATOM | 4956 | CA | VAL | B | 245 | 59.019 | -22.589 | 76.230 | 1.00 | 43.55 |
| ATOM | 4957 | CB | VAL | B | 245 | 58.867 | -22.514 | 77.771 | 1.00 | 45.89 |
| ATOM | 4958 | CG1 | VAL | B | 245 | 57.665 | -23.322 | 78.231 | 1.00 | 49.90 |
| ATOM | 4959 | CG2 | VAL | B | 245 | 60.131 | -23.040 | 78.435 | 1.00 | 46.37 |
| ATOM | 4960 | C | VAL | B | 245 | 57.727 | -22.115 | 75.565 | 1.00 | 41.01 |
| ATOM | 4961 | O | VAL | B | 245 | 56.659 | -22.676 | 75.798 | 1.00 | 39.36 |
| ATOM | 4962 | N | PHE | B | 246 | 57.814 | -21.101 | 74.716 | 1.00 | 34.37 |
| ATOM | 4963 | CA | PHE | B | 246 | 56.610 | -20.602 | 74.077 | 1.00 | 34.36 |
| ATOM | 4964 | CB | PHE | B | 246 | 55.986 | -19.517 | 74.958 | 1.00 | 30.80 |
| ATOM | 4965 | CG | PHE | B | 246 | 54.542 | -19.230 | 74.644 | 1.00 | 32.57 |
| ATOM | 4966 | CD1 | PHE | B | 246 | 53.548 | -20.142 | 74.989 | 1.00 | 27.72 |
| ATOM | 4967 | CD2 | PHE | B | 246 | 54.174 | -18.048 | 74.003 | 1.00 | 28.20 |
| ATOM | 4968 | CE1 | PHE | B | 246 | 52.207 | -19.878 | 74.704 | 1.00 | 26.71 |
| ATOM | 4969 | CE2 | PHE | B | 246 | 52.836 | -17.773 | 73.713 | 1.00 | 29.27 |
| ATOM | 4970 | CC | PHE | B | 246 | 51.850 | -18.689 | 74.065 | 1.00 | 26.18 |
| ATOM | 4971 | C | PHE | B | 246 | 56.904 | -20.040 | 72.682 | 1.00 | 35.32 |
| ATOM | 4972 | O | PHE | B | 246 | 57.740 | -19.153 | 72.517 | 1.00 | 31.73 |
| ATOM | 4973 | N | GLU | B | 247 | 56.205 | -20.568 | 71.683 | 1.00 | 37.00 |

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Figure 18-76

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 4974 | CA | GLU | B | 247 | 56.363 | -20.137 | 70.296 | 1.00 | 40.73 |
| ATOM | 4975 | CB | GLU | B | 247 | 56.518 | -21.347 | 69.370 | 1.00 | 43.38 |
| ATOM | 4976 | CG | GLU | B | 247 | 56.670 | -22.702 | 70.073 | 1.00 | 51.49 |
| ATOM | 4977 | CD | GLU | B | 247 | 55.381 | -23.214 | 70.718 | 1.00 | 55.29 |
| ATOM | 4978 | OE1 | GLU | B | 247 | 54.887 | -22.601 | 71.691 | 1.00 | 49.08 |
| ATOM | 4979 | OE2 | GLU | B | 247 | 54.859 | -24.246 | 70.241 | 1.00 | 60.95 |
| ATOM | 4980 | C | GLU | B | 247 | 55.090 | -19.379 | 69.939 | 1.00 | 39.04 |
| ATOM | 4981 | O | GLU | B | 247 | 54.129 | -19.960 | 69.436 | 1.00 | 39.49 |
| ATOM | 4982 | N | PRO | B | 248 | 55.076 | -18.064 | 70.182 | 1.00 | 35.13 |
| ATOM | 4983 | CD | PRO | B | 248 | 56.188 | -17.270 | 70.733 | 1.00 | 33.57 |
| ATOM | 4984 | CA | PRO | B | 248 | 53.935 | -17.188 | 69.916 | 1.00 | 36.03 |
| ATOM | 4985 | CB | PRO | B | 248 | 54.375 | -15.878 | 70.562 | 1.00 | 35.33 |
| ATOM | 4986 | CG | PRO | B | 248 | 55.844 | -15.880 | 70.233 | 1.00 | 32.85 |
| ATOM | 4987 | C | PRO | B | 248 | 53.563 | -16.990 | 68.457 | 1.00 | 33.44 |
| ATOM | 4988 | O | PRO | B | 248 | 54.427 | -16.808 | 67.604 | 1.00 | 29.38 |
| ATOM | 4989 | N | GLU | B | 249 | 52.263 | -17.012 | 68.182 | 1.00 | 32.23 |
| ATOM | 4990 | CA | GLU | B | 249 | 51.773 | -16.782 | 66.828 | 1.00 | 29.35 |
| ATOM | 4991 | CB | GLU | B | 249 | 50.374 | -17.366 | 66.645 | 1.00 | 31.87 |
| ATOM | 4992 | CG | GLU | B | 249 | 50.284 | -18.867 | 66.787 | 1.00 | 28.64 |
| ATOM | 4993 | CD | GLU | B | 249 | 48.847 | -19.338 | 66.747 | 1.00 | 33.37 |
| ATOM | 4994 | OE1 | GLU | B | 249 | 48.069 | -18.917 | 67.630 | 1.00 | 26.38 |
| ATOM | 4995 | OE2 | GLU | B | 249 | 48.494 | -20.115 | 65.835 | 1.00 | 37.71 |
| ATOM | 4996 | C | GLU | B | 249 | 51.700 | -15.273 | 66.650 | 1.00 | 28.25 |
| ATOM | 4997 | O | GLU | B | 249 | 51.776 | -14.765 | 65.537 | 1.00 | 21.47 |
| ATOM | 4998 | N | VAL | B | 250 | 51.561 | -14.564 | 67.768 | 1.00 | 21.77 |
| ATOM | 4999 | CA | VAL | B | 250 | 51.459 | -13.110 | 67.756 | 1.00 | 21.41 |
| ATOM | 5000 | CB | VAL | B | 250 | 50.027 | -12.676 | 67.357 | 1.00 | 26.42 |
| ATOM | 5001 | CG1 | VAL | B | 250 | 49.037 | -13.196 | 68.378 | 1.00 | 20.96 |
| ATOM | 5002 | CG2 | VAL | B | 250 | 49.931 | -11.166 | 67.243 | 1.00 | 24.68 |
| ATOM | 5003 | C | VAL | B | 250 | 51.757 | -12.608 | 69.168 | 1.00 | 22.88 |
| ATOM | 5004 | O | VAL | B | 250 | 51.592 | -13.354 | 70.133 | 1.00 | 18.00 |
| ATOM | 5005 | N | TYR | B | 251 | 52.201 | -11.359 | 69.295 | 1.00 | 20.28 |
| ATOM | 5006 | CA | TYR | B | 251 | 52.481 | -10.823 | 70.620 | 1.00 | 22.33 |
| ATOM | 5007 | CB | TYR | B | 251 | 53.956 | -11.043 | 70.999 | 1.00 | 20.67 |
| ATOM | 5008 | CG | TYR | B | 251 | 54.948 | -10.045 | 70.427 | 1.00 | 21.89 |
| ATOM | 5009 | CD1 | TYR | B | 251 | 55.198 | -8.834 | 71.072 | 1.00 | 19.31 |
| ATOM | 5010 | CE1 | TYR | B | 251 | 56.129 | -7.922 | 70.562 | 1.00 | 23.73 |
| ATOM | 5011 | CD2 | TYR | B | 251 | 55.651 | -10.321 | 69.254 | 1.00 | 18.72 |
| ATOM | 5012 | CE2 | TYR | B | 251 | 56.580 | -9.417 | 68.734 | 1.00 | 22.71 |
| ATOM | 5013 | CZ | TYR | B | 251 | 56.813 | -8.220 | 69.390 | 1.00 | 27.33 |
| ATOM | 5014 | OH | TYR | B | 251 | 57.705 | -7.308 | 68.865 | 1.00 | 23.18 |
| ATOM | 5015 | C | TYR | B | 251 | 52.134 | -9.349 | 70.732 | 1.00 | 25.71 |
| ATOM | 5016 | O | TYR | B | 251 | 52.095 | -8.622 | 69.728 | 1.00 | 20.14 |
| ATOM | 5017 | N | LEU | B | 252 | 51.834 | -8.930 | 71.958 | 1.00 | 21.13 |
| ATOM | 5018 | CA | LEU | B | 252 | 51.533 | -7.532 | 72.252 | 1.00 | 24.61 |
| ATOM | 5019 | CB | LEU | B | 252 | 50.154 | -7.373 | 72.897 | 1.00 | 22.88 |
| ATOM | 5020 | CG | LEU | B | 252 | 48.915 | -7.435 | 71.996 | 1.00 | 23.73 |
| ATOM | 5021 | CD1 | LEU | B | 252 | 48.779 | -8.792 | 71.360 | 1.00 | 23.18 |
| ATOM | 5022 | CD2 | LEU | B | 252 | 47.697 | -7.119 | 72.833 | 1.00 | 29.06 |
| ATOM | 5023 | C | LEU | B | 252 | 52.610 | -7.044 | 73.217 | 1.00 | 24.77 |
| ATOM | 5024 | O | LEU | B | 252 | 53.064 | -7.797 | 74.076 | 1.00 | 23.33 |
| ATOM | 5025 | N | LEU | B | 253 | 53.011 | -5.786 | 73.071 | 1.00 | 20.14 |
| ATOM | 5026 | CA | LEU | B | 253 | 54.057 | -5.209 | 73.911 | 1.00 | 20.33 |
| ATOM | 5027 | CB | LEU | B | 253 | 55.304 | -4.946 | 73.051 | 1.00 | 15.18 |
| ATOM | 5028 | CG | LEU | B | 253 | 56.490 | -4.210 | 73.688 | 1.00 | 18.34 |
| ATOM | 5029 | CD1 | LEU | B | 253 | 57.062 | -5.044 | 74.829 | 1.00 | 14.11 |
| ATOM | 5030 | CD2 | LEU | B | 253 | 57.552 | -3.953 | 72.624 | 1.00 | 19.60 |
| ATOM | 5031 | C | LEU | B | 253 | 53.550 | -3.913 | 74.536 | 1.00 | 20.54 |
| ATOM | 5032 | O | LEU | B | 253 | 53.200 | -2.974 | 73.821 | 1.00 | 22.80 |
| ATOM | 5033 | N | GLN | B | 254 | 53.495 | -3.858 | 75.865 | 1.00 | 20.37 |
| ATOM | 5034 | CA | GLN | B | 254 | 53.000 | -2.654 | 76.539 | 1.00 | 21.77 |
| ATOM | 5035 | CB | GLN | B | 254 | 52.129 | -3.040 | 77.755 | 1.00 | 17.85 |
| ATOM | 5036 | CG | GLN | B | 254 | 52.724 | -2.815 | 79.124 | 1.00 | 32.51 |
| ATOM | 5037 | CD | GLN | B | 254 | 52.563 | -1.396 | 79.609 | 1.00 | 28.19 |
| ATOM | 5038 | OE1 | GLN | B | 254 | 51.507 | -0.996 | 80.124 | 1.00 | 26.96 |
| ATOM | 5039 | NE2 | GLN | B | 254 | 53.603 | -0.619 | 79.432 | 1.00 | 16.80 |

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Figure 18-77

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5040 | C | GLN | B | 254 | 54.211 | -1.793 | 76.887 | 1.00 | 20.15 |
| ATOM | 5041 | O | GLN | B | 254 | 55.186 | -2.254 | 77.497 | 1.00 | 20.11 |
| ATOM | 5042 | N | LEU | B | 255 | 54.146 | -0.532 | 76.468 | 1.00 | 19.46 |
| ATOM | 5043 | CA | LEU | B | 255 | 55.268 | 0.386 | 76.614 | 1.00 | 15.99 |
| ATOM | 5044 | CB | LEU | B | 255 | 55.692 | 0.831 | 75.211 | 1.00 | 18.15 |
| ATOM | 5045 | CG | LEU | B | 255 | 56.143 | -0.316 | 74.296 | 1.00 | 21.80 |
| ATOM | 5046 | CD1 | LEU | B | 255 | 56.215 | 0.159 | 72.850 | 1.00 | 16.70 |
| ATOM | 5047 | CD2 | LEU | B | 255 | 57.501 | -0.843 | 74.771 | 1.00 | 13.76 |
| ATOM | 5048 | C | LEU | B | 255 | 55.083 | 1.614 | 77.492 | 1.00 | 21.41 |
| ATOM | 5049 | O | LEU | B | 255 | 55.379 | 2.741 | 77.065 | 1.00 | 18.40 |
| ATOM | 5050 | N | GLY | B | 256 | 54.618 | 1.408 | 78.718 | 1.00 | 16.80 |
| ATOM | 5051 | CA | GLY | B | 256 | 54.456 | 2.519 | 79.634 | 1.00 | 19.90 |
| ATOM | 5052 | C | GLY | B | 256 | 55.816 | 3.181 | 79.818 | 1.00 | 17.68 |
| ATOM | 5053 | O | GLY | B | 256 | 56.854 | 2.514 | 79.841 | 1.00 | 13.96 |
| ATOM | 5054 | N | THR | B | 257 | 55.824 | 4.497 | 79.936 | 1.00 | 19.55 |
| ATOM | 5055 | CA | THR | B | 257 | 57.081 | 5.205 | 80.098 | 1.00 | 19.47 |
| ATOM | 5056 | CB | THR | B | 257 | 57.044 | 6.547 | 79.340 | 1.00 | 21.49 |
| ATOM | 5057 | OG1 | THR | B | 257 | 55.989 | 7.365 | 79.858 | 1.00 | 17.43 |
| ATOM | 5058 | CG2 | THR | B | 257 | 56.780 | 6.311 | 77.850 | 1.00 | 22.49 |
| ATOM | 5059 | C | THR | B | 257 | 57.440 | 5.466 | 81.564 | 1.00 | 20.75 |
| ATOM | 5060 | O | THR | B | 257 | 58.480 | 6.054 | 81.843 | 1.00 | 25.01 |
| ATOM | 5061 | N | ASP | B | 258 | 56.618 | 5.004 | 82.504 | 1.00 | 17.23 |
| ATOM | 5062 | CA | ASP | B | 258 | 56.929 | 5.277 | 83.906 | 1.00 | 17.42 |
| ATOM | 5063 | CB | ASP | B | 258 | 55.744 | 4.940 | 84.846 | 1.00 | 12.75 |
| ATOM | 5064 | CG | ASP | B | 258 | 55.197 | 3.524 | 84.676 | 1.00 | 21.60 |
| ATOM | 5065 | C | ASP | B | 258 | 58.245 | 4.718 | 84.460 | 1.00 | 16.09 |
| ATOM | 5066 | O | ASP | B | 258 | 58.667 | 5.116 | 85.542 | 1.00 | 22.07 |
| ATOM | 5067 | OD1 | ASP | B | 258 | 55.901 | 2.642 | 84.150 | 1.00 | 17.74 |
| ATOM | 5068 | OD2 | ASP | B | 258 | 54.041 | 3.281 | 85.109 | 1.00 | 18.68 |
| ATOM | 5069 | N | PRO | B | 259 | 58.879 | 3.746 | 83.779 | 1.00 | 20.98 |
| ATOM | 5070 | CD | PRO | B | 259 | 58.474 | 2.901 | 82.641 | 1.00 | 17.75 |
| ATOM | 5071 | CA | PRO | B | 259 | 60.154 | 3.257 | 84.321 | 1.00 | 22.63 |
| ATOM | 5072 | CB | PRO | B | 259 | 60.395 | 1.988 | 83.506 | 1.00 | 23.46 |
| ATOM | 5073 | CG | PRO | B | 259 | 59.800 | 2.343 | 82.199 | 1.00 | 27.08 |
| ATOM | 5074 | C | PRO | B | 259 | 61.305 | 4.284 | 84.172 | 1.00 | 23.86 |
| ATOM | 5075 | O | PRO | B | 259 | 62.406 | 4.082 | 84.698 | 1.00 | 24.24 |
| ATOM | 5076 | N | LEU | B | 260 | 61.054 | 5.387 | 83.465 | 1.00 | 20.49 |
| ATOM | 5077 | CA | LEU | B | 260 | 62.080 | 6.417 | 83.262 | 1.00 | 15.17 |
| ATOM | 5078 | CB | LEU | B | 260 | 61.626 | 7.408 | 82.185 | 1.00 | 17.03 |
| ATOM | 5079 | CG | LEU | B | 260 | 61.431 | 6.881 | 80.760 | 1.00 | 16.02 |
| ATOM | 5080 | CD1 | LEU | B | 260 | 60.703 | 7.915 | 79.901 | 1.00 | 17.03 |
| ATOM | 5081 | CD2 | LEU | B | 260 | 62.803 | 6.546 | 80.163 | 1.00 | 18.58 |
| ATOM | 5082 | C | LEU | B | 260 | 62.449 | 7.194 | 84.541 | 1.00 | 22.45 |
| ATOM | 5083 | O | LEU | B | 260 | 61.611 | 7.440 | 85.412 | 1.00 | 17.84 |
| ATOM | 5084 | N | LEU | B | 261 | 63.713 | 7.588 | 84.635 | 1.00 | 22.90 |
| ATOM | 5085 | CA | LEU | B | 261 | 64.219 | 8.332 | 85.782 | 1.00 | 26.34 |
| ATOM | 5086 | CB | LEU | B | 261 | 65.605 | 8.914 | 85.473 | 1.00 | 20.58 |
| ATOM | 5087 | CG | LEU | B | 261 | 66.180 | 9.850 | 86.553 | 1.00 | 28.44 |
| ATOM | 5088 | CD1 | LEU | B | 261 | 66.481 | 9.055 | 87.812 | 1.00 | 29.84 |
| ATOM | 5089 | CD2 | LEU | B | 261 | 67.462 | 10.522 | 86.057 | 1.00 | 32.10 |
| ATOM | 5090 | C | LEU | B | 261 | 63.315 | 9.475 | 86.227 | 1.00 | 27.61 |
| ATOM | 5091 | O | LEU | B | 261 | 62.978 | 9.586 | 87.408 | 1.00 | 24.02 |
| ATOM | 5092 | N | GLU | B | 262 | 62.934 | 10.315 | 85.269 | 1.00 | 23.33 |
| ATOM | 5093 | CA | GLU | B | 262 | 62.126 | 11.490 | 85.530 | 1.00 | 23.38 |
| ATOM | 5094 | CB | GLU | B | 262 | 62.115 | 12.415 | 84.302 | 1.00 | 23.17 |
| ATOM | 5095 | CG | GLU | B | 262 | 63.503 | 12.854 | 83.806 | 1.00 | 28.98 |
| ATOM | 5096 | CD | GLU | B | 262 | 64.179 | 11.831 | 82.902 | 1.00 | 32.26 |
| ATOM | 5097 | OE1 | GLU | B | 262 | 63.702 | 10.673 | 82.838 | 1.00 | 29.28 |
| ATOM | 5098 | OE2 | GLU | B | 262 | 65.201 | 12.186 | 82.264 | 1.00 | 25.42 |
| ATOM | 5099 | C | GLU | B | 262 | 60.693 | 11.249 | 85.976 | 1.00 | 23.25 |
| ATOM | 5100 | O | GLU | B | 262 | 60.013 | 12.192 | 86.368 | 1.00 | 27.63 |
| ATOM | 5101 | N | ASP | B | 263 | 60.219 | 10.011 | 85.927 | 1.00 | 22.25 |
| ATOM | 5102 | CA | ASP | B | 263 | 58.840 | 9.751 | 86.345 | 1.00 | 24.46 |
| ATOM | 5103 | CB | ASP | B | 263 | 58.214 | 8.659 | 85.465 | 1.00 | 20.94 |
| ATOM | 5104 | CG | ASP | B | 263 | 56.710 | 8.543 | 85.659 | 1.00 | 25.30 |
| ATOM | 5105 | OD1 | ASP | B | 263 | 55.995 | 8.318 | 84.656 | 1.00 | 21.82 |

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Figure 18-78

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5106 | OD2 | ASP | B | 263 | 56.239 | 8.666 | 86.811 | 1.00 | 18.31 |
| ATOM | 5107 | C | ASP | B | 263 | 58.834 | 9.339 | 87.814 | 1.00 | 26.39 |
| ATOM | 5108 | O | ASP | B | 263 | 59.437 | 8.335 | 88.179 | 1.00 | 22.11 |
| ATOM | 5109 | N | TYR | B | 264 | 58.155 | 10.124 | 88.648 | 1.00 | 25.81 |
| ATOM | 5110 | CA | TYR | B | 264 | 58.101 | 9.864 | 90.084 | 1.00 | 30.96 |
| ATOM | 5111 | CB | TYR | B | 264 | 57.511 | 11.055 | 90.841 | 1.00 | 36.80 |
| ATOM | 5112 | CG | TYR | B | 264 | 58.241 | 12.356 | 90.645 | 1.00 | 46.58 |
| ATOM | 5113 | CD1 | TYR | B | 264 | 57.981 | 13.166 | 89.542 | 1.00 | 47.03 |
| ATOM | 5114 | CE1 | TYR | B | 264 | 58.654 | 14.370 | 89.364 | 1.00 | 50.25 |
| ATOM | 5115 | CD2 | TYR | B | 264 | 59.197 | 12.779 | 91.565 | 1.00 | 50.94 |
| ATOM | 5116 | CE2 | TYR | B | 264 | 59.876 | 13.977 | 91.396 | 1.00 | 51.28 |
| ATOM | 5117 | CZ | TYR | B | 264 | 59.600 | 14.769 | 90.297 | 1.00 | 52.21 |
| ATOM | 5118 | OH | TYR | B | 264 | 60.268 | 15.961 | 90.142 | 1.00 | 49.65 |
| ATOM | 5119 | C | TYR | B | 264 | 57.340 | 8.628 | 90.525 | 1.00 | 31.04 |
| ATOM | 5120 | O | TYR | B | 264 | 57.514 | 8.181 | 91.657 | 1.00 | 24.50 |
| ATOM | 5121 | N | LEU | B | 265 | 56.491 | 8.074 | 89.666 | 1.00 | 26.68 |
| ATOM | 5122 | CA | LEU | B | 265 | 55.744 | 6.900 | 90.086 | 1.00 | 24.17 |
| ATOM | 5123 | CB | LEU | B | 265 | 54.371 | 6.838 | 89.390 | 1.00 | 24.69 |
| ATOM | 5124 | CG | LEU | B | 265 | 53.415 | 7.982 | 89.761 | 1.00 | 26.00 |
| ATOM | 5125 | CD1 | LEU | B | 265 | 51.970 | 7.583 | 89.460 | 1.00 | 22.21 |
| ATOM | 5126 | CD2 | LEU | B | 265 | 53.530 | 8.281 | 91.238 | 1.00 | 29.31 |
| ATOM | 5127 | C | LEU | B | 265 | 56.478 | 5.568 | 89.948 | 1.00 | 25.83 |
| ATOM | 5128 | O | LEU | B | 265 | 55.848 | 4.512 | 89.908 | 1.00 | 21.74 |
| ATOM | 5129 | N | SER | B | 266 | 57.808 | 5.618 | 89.867 | 1.00 | 23.30 |
| ATOM | 5130 | CA | SER | B | 266 | 58.608 | 4.398 | 89.813 | 1.00 | 20.75 |
| ATOM | 5131 | CB | SER | B | 266 | 58.820 | 3.900 | 88.378 | 1.00 | 19.67 |
| ATOM | 5132 | OG | SER | B | 266 | 59.863 | 4.615 | 87.739 | 1.00 | 18.11 |
| ATOM | 5133 | C | SER | B | 266 | 59.963 | 4.710 | 90.420 | 1.00 | 23.01 |
| ATOM | 5134 | O | SER | B | 266 | 60.437 | 5.845 | 90.345 | 1.00 | 17.74 |
| ATOM | 5135 | N | LYS | B | 267 | 60.590 | 3.707 | 91.023 | 1.00 | 24.25 |
| ATOM | 5136 | CA | LYS | B | 267 | 61.905 | 3.916 | 91.613 | 1.00 | 23.79 |
| ATOM | 5137 | CB | LYS | B | 267 | 62.027 | 3.153 | 92.929 | 1.00 | 23.71 |
| ATOM | 5138 | CG | LYS | B | 267 | 60.989 | 3.582 | 93.960 | 1.00 | 27.29 |
| ATOM | 5139 | CD | LYS | B | 267 | 61.059 | 5.088 | 94.207 | 1.00 | 30.33 |
| ATOM | 5140 | CE | LYS | B | 267 | 60.067 | 5.535 | 95.273 | 1.00 | 30.90 |
| ATOM | 5141 | NZ | LYS | B | 267 | 60.155 | 7.004 | 95.509 | 1.00 | 33.37 |
| ATOM | 5142 | C | LYS | B | 267 | 62.990 | 3.483 | 90.634 | 1.00 | 26.41 |
| ATOM | 5143 | O | LYS | B | 267 | 64.153 | 3.317 | 91.016 | 1.00 | 25.33 |
| ATOM | 5144 | N | PHE | B | 268 | 62.595 | 3.288 | 89.375 | 1.00 | 22.18 |
| ATOM | 5145 | CA | PHE | B | 268 | 63.529 | 2.919 | 88.318 | 1.00 | 22.78 |
| ATOM | 5146 | CB | PHE | B | 268 | 62.814 | 2.171 | 87.179 | 1.00 | 20.55 |
| ATOM | 5147 | CG | PHE | B | 268 | 62.389 | 0.761 | 87.526 | 1.00 | 19.23 |
| ATOM | 5148 | CD1 | PHE | B | 268 | 61.722 | -0.025 | 86.585 | 1.00 | 20.72 |
| ATOM | 5149 | CD2 | PHE | B | 268 | 62.673 | 0.207 | 88.773 | 1.00 | 18.17 |
| ATOM | 5150 | CE1 | PHE | B | 268 | 61.344 | -1.336 | 86.875 | 1.00 | 18.83 |
| ATOM | 5151 | CE2 | PHE | B | 268 | 62.300 | -1.105 | 89.073 | 1.00 | 20.05 |
| ATOM | 5152 | CZ | PHE | B | 268 | 61.634 | -1.879 | 88.122 | 1.00 | 19.70 |
| ATOM | 5153 | C | PHE | B | 268 | 64.114 | 4.222 | 87.785 | 1.00 | 23.66 |
| ATOM | 5154 | O | PHE | B | 268 | 63.412 | 5.232 | 87.692 | 1.00 | 19.40 |
| ATOM | 5155 | N | ASN | B | 269 | 65.396 | 4.203 | 87.437 | 1.00 | 21.96 |
| ATOM | 5156 | CA | ASN | B | 269 | 66.060 | 5.396 | 86.926 | 1.00 | 25.04 |
| ATOM | 5157 | CB | ASN | B | 269 | 67.243 | 5.783 | 87.824 | 1.00 | 25.68 |
| ATOM | 5158 | CG | ASN | B | 269 | 66.845 | 5.946 | 89.273 | 1.00 | 27.04 |
| ATOM | 5159 | OD1 | ASN | B | 269 | 65.832 | 6.557 | 89.579 | 1.00 | 28.81 |
| ATOM | 5160 | ND2 | ASN | B | 269 | 67.659 | 5.419 | 90.176 | 1.00 | 31.12 |
| ATOM | 5161 | C | ASN | B | 269 | 66.579 | 5.151 | 85.523 | 1.00 | 25.87 |
| ATOM | 5162 | O | ASN | B | 269 | 67.769 | 5.336 | 85.268 | 1.00 | 24.58 |
| ATOM | 5163 | N | LEU | B | 270 | 65.695 | 4.757 | 84.611 | 1.00 | 21.37 |
| ATOM | 5164 | CA | LEU | B | 270 | 66.116 | 4.462 | 83.241 | 1.00 | 16.35 |
| ATOM | 5165 | CB | LEU | B | 270 | 65.176 | 3.426 | 82.610 | 1.00 | 24.12 |
| ATOM | 5166 | CG | LEU | B | 270 | 64.909 | 2.144 | 83.412 | 1.00 | 27.89 |
| ATOM | 5167 | CD1 | LEU | B | 270 | 64.181 | 1.136 | 82.515 | 1.00 | 23.01 |
| ATOM | 5168 | CD2 | LEU | B | 270 | 66.221 | 1.547 | 83.904 | 1.00 | 23.92 |
| ATOM | 5169 | C | LEU | B | 270 | 66.184 | 5.682 | 82.337 | 1.00 | 20.06 |
| ATOM | 5170 | O | LEU | B | 270 | 65.654 | 6.761 | 82.663 | 1.00 | 16.34 |
| ATOM | 5171 | N | SER | B | 271 | 66.839 | 5.497 | 81.193 | 1.00 | 20.07 |

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Figure 18-79

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5172 | CA | SER | B | 271 | 66.989 | 6.546 | 80.200 | 1.00 | 21.20 |
| ATOM | 5173 | CB | SER | B | 271 | 68.437 | 6.621 | 79.714 | 1.00 | 21.80 |
| ATOM | 5174 | OG | SER | B | 271 | 68.772 | 5.485 | 78.921 | 1.00 | 21.47 |
| ATOM | 5175 | C | SER | B | 271 | 66.106 | 6.228 | 79.000 | 1.00 | 22.83 |
| ATOM | 5176 | O | SER | B | 271 | 65.631 | 5.102 | 78.854 | 1.00 | 16.12 |
| ATOM | 5177 | N | ASN | B | 272 | 65.916 | 7.238 | 78.154 | 1.00 | 20.84 |
| ATOM | 5178 | CA | ASN | B | 272 | 65.152 | 7.156 | 76.906 | 1.00 | 27.82 |
| ATOM | 5179 | CB | ASN | B | 272 | 65.263 | 8.478 | 76.123 | 1.00 | 30.30 |
| ATOM | 5180 | CG | ASN | B | 272 | 64.198 | 9.456 | 76.475 | 1.00 | 37.83 |
| ATOM | 5181 | OD1 | ASN | B | 272 | 64.167 | 10.575 | 75.946 | 1.00 | 37.72 |
| ATOM | 5182 | ND2 | ASN | B | 272 | 63.299 | 9.052 | 77.360 | 1.00 | 41.69 |
| ATOM | 5183 | C | ASN | B | 272 | 65.701 | 6.088 | 75.974 | 1.00 | 26.88 |
| ATOM | 5184 | O | ASN | B | 272 | 64.967 | 5.280 | 75.412 | 1.00 | 23.12 |
| ATOM | 5185 | N | VAL | B | 273 | 67.012 | 6.160 | 75.774 | 1.00 | 20.40 |
| ATOM | 5186 | CA | VAL | B | 273 | 67.745 | 5.260 | 74.899 | 1.00 | 27.34 |
| ATOM | 5187 | CB | VAL | B | 273 | 69.225 | 5.705 | 74.805 | 1.00 | 30.40 |
| ATOM | 5188 | CG1 | VAL | B | 273 | 70.036 | 4.691 | 74.029 | 1.00 | 34.98 |
| ATOM | 5189 | CG2 | VAL | B | 273 | 69.299 | 7.057 | 74.115 | 1.00 | 33.57 |
| ATOM | 5190 | C | VAL | B | 273 | 67.664 | 3.812 | 75.343 | 1.00 | 24.23 |
| ATOM | 5191 | O | VAL | B | 273 | 67.590 | 2.913 | 74.513 | 1.00 | 24.19 |
| ATOM | 5192 | N | ALA | B | 274 | 67.690 | 3.580 | 76.648 | 1.00 | 20.96 |
| ATOM | 5193 | CA | ALA | B | 274 | 67.589 | 2.220 | 77.151 | 1.00 | 18.12 |
| ATOM | 5194 | CB | ALA | B | 274 | 67.858 | 2.195 | 78.646 | 1.00 | 19.09 |
| ATOM | 5195 | C | ALA | B | 274 | 66.172 | 1.729 | 76.863 | 1.00 | 18.23 |
| ATOM | 5196 | O | ALA | B | 274 | 65.962 | 0.567 | 76.525 | 1.00 | 20.77 |
| ATOM | 5197 | N | PHE | B | 275 | 65.207 | 2.631 | 77.003 | 1.00 | 18.50 |
| ATOM | 5198 | CA | PHE | B | 275 | 63.802 | 2.310 | 76.761 | 1.00 | 21.25 |
| ATOM | 5199 | CB | PHE | B | 275 | 62.941 | 3.546 | 77.037 | 1.00 | 22.24 |
| ATOM | 5200 | CG | PHE | B | 275 | 61.466 | 3.303 | 76.921 | 1.00 | 24.72 |
| ATOM | 5201 | CD1 | PHE | B | 275 | 60.815 | 2.483 | 77.826 | 1.00 | 23.64 |
| ATOM | 5202 | CD2 | PHE | B | 275 | 60.732 | 3.893 | 75.907 | 1.00 | 27.31 |
| ATOM | 5203 | CE1 | PHE | B | 275 | 59.450 | 2.254 | 77.722 | 1.00 | 27.82 |
| ATOM | 5204 | CE2 | PHE | B | 275 | 59.365 | 3.670 | 75.795 | 1.00 | 27.62 |
| ATOM | 5205 | CZ | PHE | B | 275 | 58.727 | 2.851 | 76.701 | 1.00 | 25.78 |
| ATOM | 5206 | C | PHE | B | 275 | 63.642 | 1.860 | 75.305 | 1.00 | 24.47 |
| ATOM | 5207 | O | PHE | B | 275 | 63.045 | 0.821 | 75.030 | 1.00 | 22.68 |
| ATOM | 5208 | N | LEU | B | 276 | 64.183 | 2.648 | 74.378 | 1.00 | 23.85 |
| ATOM | 5209 | CA | LEU | B | 276 | 64.128 | 2.330 | 72.946 | 1.00 | 21.28 |
| ATOM | 5210 | CB | LEU | B | 276 | 64.814 | 3.421 | 72.134 | 1.00 | 19.87 |
| ATOM | 5211 | CG | LEU | B | 276 | 65.114 | 3.132 | 70.662 | 1.00 | 24.94 |
| ATOM | 5212 | CD1 | LEU | B | 276 | 63.818 | 2.852 | 69.936 | 1.00 | 24.81 |
| ATOM | 5213 | CD2 | LEU | B | 276 | 65.840 | 4.312 | 70.018 | 1.00 | 21.01 |
| ATOM | 5214 | C | LEU | B | 276 | 64.841 | 1.021 | 72.653 | 1.00 | 22.33 |
| ATOM | 5215 | O | LEU | B | 276 | 64.348 | 0.191 | 71.886 | 1.00 | 20.73 |
| ATOM | 5216 | N | LYS | B | 277 | 66.011 | 0.857 | 73.261 | 1.00 | 20.72 |
| ATOM | 5217 | CA | LYS | B | 277 | 66.823 | -0.335 | 73.076 | 1.00 | 24.36 |
| ATOM | 5218 | CB | LYS | B | 277 | 68.086 | -0.239 | 73.938 | 1.00 | 27.37 |
| ATOM | 5219 | CG | LYS | B | 277 | 69.303 | -0.973 | 73.381 | 1.00 | 35.58 |
| ATOM | 5220 | CD | LYS | B | 277 | 69.061 | -2.456 | 73.188 | 1.00 | 43.87 |
| ATOM | 5221 | CE | LYS | B | 277 | 70.283 | -3.137 | 72.580 | 1.00 | 44.87 |
| ATOM | 5222 | NZ | LYS | B | 277 | 70.616 | -2.586 | 71.230 | 1.00 | 49.66 |
| ATOM | 5223 | C | LYS | B | 277 | 66.000 | -1.554 | 73.482 | 1.00 | 24.22 |
| ATOM | 5224 | O | LYS | B | 277 | 65.987 | -2.568 | 72.777 | 1.00 | 19.90 |
| ATOM | 5225 | N | ALA | B | 278 | 65.319 | -1.454 | 74.624 | 1.00 | 22.32 |
| ATOM | 5226 | CA | ALA | B | 278 | 64.476 | -2.544 | 75.114 | 1.00 | 21.71 |
| ATOM | 5227 | CB | ALA | B | 278 | 63.752 | -2.117 | 76.381 | 1.00 | 17.34 |
| ATOM | 5228 | C | ALA | B | 278 | 63.459 | -2.896 | 74.031 | 1.00 | 22.68 |
| ATOM | 5229 | O | ALA | B | 278 | 63.231 | -4.068 | 73.723 | 1.00 | 19.27 |
| ATOM | 5230 | N | PHE | B | 279 | 62.849 | -1.862 | 73.464 | 1.00 | 24.79 |
| ATOM | 5231 | CA | PHE | B | 279 | 61.860 | -2.014 | 72.398 | 1.00 | 22.74 |
| ATOM | 5232 | CB | PHE | B | 279 | 61.395 | -0.629 | 71.955 | 1.00 | 22.46 |
| ATOM | 5233 | CG | PHE | B | 279 | 60.467 | -0.640 | 70.778 | 1.00 | 22.62 |
| ATOM | 5234 | CD1 | PHE | B | 279 | 59.196 | -1.182 | 70.882 | 1.00 | 21.74 |
| ATOM | 5235 | CD2 | PHE | B | 279 | 60.862 | -0.078 | 69.567 | 1.00 | 26.07 |
| ATOM | 5236 | CE1 | PHE | B | 279 | 58.325 | -1.162 | 69.799 | 1.00 | 27.02 |
| ATOM | 5237 | CE2 | PHE | B | 279 | 60.001 | -0.051 | 68.476 | 1.00 | 25.57 |

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Figure 18-80

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 5238 | CZ | PHE | B | 279 | 58.727 | -0.594 | 68.592 | 1.00 | 25.13 |
| ATOM | 5239 | C | PHE | B | 279 | 62.472 | -2.768 | 71.212 | 1.00 | 23.60 |
| ATOM | 5240 | O | PHE | B | 279 | 61.866 | -3.697 | 70.678 | 1.00 | 26.54 |
| ATOM | 5241 | N | ASN | B | 280 | 63.677 | -2.376 | 70.804 | 1.00 | 21.93 |
| ATOM | 5242 | CA | ASN | B | 280 | 64.318 | -3.046 | 69.680 | 1.00 | 23.70 |
| ATOM | 5243 | CB | ASN | B | 280 | 65.520 | -2.248 | 69.164 | 1.00 | 22.63 |
| ATOM | 5244 | CG | ASN | B | 280 | 65.107 | -0.937 | 68.505 | 1.00 | 30.83 |
| ATOM | 5245 | OD1 | ASN | B | 280 | 64.094 | -0.878 | 67.796 | 1.00 | 25.81 |
| ATOM | 5246 | ND2 | ASN | B | 280 | 65.900 | 0.112 | 68.714 | 1.00 | 26.54 |
| ATOM | 5247 | C | ASN | B | 280 | 64.746 | -4.466 | 70.009 | 1.00 | 26.10 |
| ATOM | 5248 | O | ASN | B | 280 | 64.775 | -5.321 | 69.124 | 1.00 | 26.16 |
| ATOM | 5249 | N | ILE | B | 281 | 65.080 | -4.724 | 71.272 | 1.00 | 26.10 |
| ATOM | 5250 | CA | ILE | B | 281 | 65.485 | -6.067 | 71.667 | 1.00 | 25.81 |
| ATOM | 5251 | CB | ILE | B | 281 | 66.006 | -6.098 | 73.124 | 1.00 | 28.50 |
| ATOM | 5252 | CG2 | ILE | B | 281 | 66.046 | -7.527 | 73.648 | 1.00 | 28.53 |
| ATOM | 5253 | CG1 | ILE | B | 281 | 67.392 | -5.454 | 73.173 | 1.00 | 32.07 |
| ATOM | 5254 | CD1 | ILE | B | 281 | 68.038 | -5.442 | 74.541 | 1.00 | 28.24 |
| ATOM | 5255 | C | ILE | B | 281 | 64.320 | -7.030 | 71.507 | 1.00 | 25.77 |
| ATOM | 5256 | O | ILE | B | 281 | 64.484 | -8.131 | 70.982 | 1.00 | 23.39 |
| ATOM | 5257 | N | VAL | B | 282 | 63.139 | -6.618 | 71.950 | 1.00 | 21.30 |
| ATOM | 5258 | CA | VAL | B | 282 | 61.961 | -7.465 | 71.813 | 1.00 | 22.90 |
| ATOM | 5259 | CB | VAL | B | 282 | 60.703 | -6.775 | 72.387 | 1.00 | 24.07 |
| ATOM | 5260 | CG1 | VAL | B | 282 | 59.464 | -7.611 | 72.093 | 1.00 | 22.28 |
| ATOM | 5261 | CG2 | VAL | B | 282 | 60.865 | -6.587 | 73.906 | 1.00 | 26.89 |
| ATOM | 5262 | C | VAL | B | 282 | 61.718 | -7.795 | 70.339 | 1.00 | 23.87 |
| ATOM | 5263 | O | VAL | B | 282 | 61.462 | -8.949 | 69.978 | 1.00 | 22.65 |
| ATOM | 5264 | N | ARG | B | 283 | 61.799 | -6.779 | 69.488 | 1.00 | 23.19 |
| ATOM | 5265 | CA | ARG | B | 283 | 61.576 | -6.971 | 68.060 | 1.00 | 27.95 |
| ATOM | 5266 | CB | ARG | B | 283 | 61.510 | -5.612 | 67.359 | 1.00 | 25.48 |
| ATOM | 5267 | CG | ARG | B | 283 | 60.337 | -4.760 | 67.838 | 1.00 | 26.55 |
| ATOM | 5268 | CD | ARG | B | 283 | 60.442 | -3.333 | 67.339 | 1.00 | 31.52 |
| ATOM | 5269 | NE | ARG | B | 283 | 60.210 | -3.208 | 65.908 | 1.00 | 24.43 |
| ATOM | 5270 | CZ | ARG | B | 283 | 60.915 | -2.414 | 65.116 | 1.00 | 26.45 |
| ATOM | 5271 | NH1 | ARG | B | 283 | 61.902 | -1.676 | 65.622 | 1.00 | 26.04 |
| ATOM | 5272 | NH2 | ARG | B | 283 | 60.634 | -2.356 | 63.825 | 1.00 | 29.64 |
| ATOM | 5273 | C | ARG | B | 283 | 62.634 | -7.855 | 67.402 | 1.00 | 32.04 |
| ATOM | 5274 | O | ARG | B | 283 | 62.341 | -8.552 | 66.431 | 1.00 | 29.76 |
| ATOM | 5275 | N | GLU | B | 284 | 63.859 | -7.821 | 67.923 | 1.00 | 31.50 |
| ATOM | 5276 | CA | GLU | B | 284 | 64.934 | -8.646 | 67.381 | 1.00 | 32.42 |
| ATOM | 5277 | CB | GLU | B | 284 | 66.289 | -8.260 | 67.992 | 1.00 | 38.31 |
| ATOM | 5278 | CG | GLU | B | 284 | 66.798 | -6.864 | 67.640 | 1.00 | 48.93 |
| ATOM | 5279 | CD | GLU | B | 284 | 68.102 | -6.518 | 68.362 | 1.00 | 56.28 |
| ATOM | 5280 | OE1 | GLU | B | 284 | 69.084 | -7.281 | 68.222 | 1.00 | 57.37 |
| ATOM | 5281 | OE2 | GLU | B | 284 | 68.150 | -5.485 | 69.069 | 1.00 | 55.42 |
| ATOM | 5282 | C | GLU | B | 284 | 64.638 | -10.105 | 67.714 | 1.00 | 31.93 |
| ATOM | 5283 | O | GLU | B | 284 | 64.899 | -11.001 | 66.913 | 1.00 | 28.26 |
| ATOM | 5284 | N | VAL | B | 285 | 64.089 | -10.340 | 68.901 | 1.00 | 28.09 |
| ATOM | 5285 | CA | VAL | B | 285 | 63.765 | -11.697 | 69.325 | 1.00 | 30.67 |
| ATOM | 5286 | CB | VAL | B | 285 | 63.687 | -11.802 | 70.863 | 1.00 | 28.33 |
| ATOM | 5287 | CG1 | VAL | B | 285 | 63.257 | -13.206 | 71.262 | 1.00 | 29.84 |
| ATOM | 5288 | CG2 | VAL | B | 285 | 65.037 | -11.470 | 71.478 | 1.00 | 26.93 |
| ATOM | 5289 | C | VAL | B | 285 | 62.460 | -12.265 | 68.758 | 1.00 | 31.19 |
| ATOM | 5290 | O | VAL | B | 285 | 62.422 | -13.423 | 68.349 | 1.00 | 31.38 |
| ATOM | 5291 | N | PHE | B | 286 | 61.398 | -11.460 | 68.729 | 1.00 | 28.21 |
| ATOM | 5292 | CA | PHE | B | 286 | 60.105 | -11.948 | 68.249 | 1.00 | 25.71 |
| ATOM | 5293 | CB | PHE | B | 286 | 59.064 | -11.853 | 69.374 | 1.00 | 24.57 |
| ATOM | 5294 | CG | PHE | B | 286 | 59.311 | -12.804 | 70.514 | 1.00 | 26.87 |
| ATOM | 5295 | CD1 | PHE | B | 286 | 59.651 | -12.331 | 71.779 | 1.00 | 25.16 |
| ATOM | 5296 | CD2 | PHE | B | 286 | 59.205 | -14.180 | 70.319 | 1.00 | 22.51 |
| ATOM | 5297 | CE1 | PHE | B | 286 | 59.880 | -13.213 | 72.833 | 1.00 | 22.92 |
| ATOM | 5298 | CE2 | PHE | B | 286 | 59.433 | -15.063 | 71.362 | 1.00 | 21.99 |
| ATOM | 5299 | CZ | PHE | B | 286 | 59.772 | -14.578 | 72.626 | 1.00 | 26.75 |
| ATOM | 5300 | C | PHE | B | 286 | 59.518 | -11.318 | 66.993 | 1.00 | 25.90 |
| ATOM | 5301 | O | PHE | B | 286 | 58.388 | -11.630 | 66.620 | 1.00 | 22.84 |
| ATOM | 5302 | N | GLY | B | 287 | 60.272 | -10.451 | 66.329 | 1.00 | 28.27 |
| ATOM | 5303 | CA | GLY | B | 287 | 59.756 | -9.814 | 65.130 | 1.00 | 23.38 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-81

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 5304 | C | GLY B 287 | 58.765 | -8.719 | 65.498 | 1.00 | 29.17 |
| ATOM | 5305 | O | GLY B 287 | 58.786 | -8.216 | 66.617 | 1.00 | 22.88 |
| ATOM | 5306 | N | GLU B 288 | 57.896 | -8.361 | 64.558 | 1.00 | 26.77 |
| ATOM | 5307 | CA | GLU B 288 | 56.893 | -7.324 | 64.754 | 1.00 | 25.38 |
| ATOM | 5308 | CB | GLU B 288 | 56.405 | -6.791 | 63.405 | 1.00 | 29.51 |
| ATOM | 5309 | CG | GLU B 288 | 57.430 | -6.003 | 62.605 | 1.00 | 36.06 |
| ATOM | 5310 | CD | GLU B 288 | 57.906 | -4.769 | 63.347 | 1.00 | 41.10 |
| ATOM | 5311 | OE1 | GLU B 288 | 57.058 | -4.055 | 63.919 | 1.00 | 41.19 |
| ATOM | 5312 | OE2 | GLU B 288 | 59.125 | -4.503 | 63.348 | 1.00 | 44.69 |
| ATOM | 5313 | C | GLU B 288 | 55.682 | -7.819 | 65.527 | 1.00 | 27.87 |
| ATOM | 5314 | O | GLU B 288 | 55.209 | -8.931 | 65.308 | 1.00 | 26.80 |
| ATOM | 5315 | N | GLY B 289 | 55.176 | -6.973 | 66.419 | 1.00 | 24.53 |
| ATOM | 5316 | CA | GLY B 289 | 54.006 | -7.326 | 67.204 | 1.00 | 29.17 |
| ATOM | 5317 | C | GLY B 289 | 53.015 | -6.171 | 67.244 | 1.00 | 30.46 |
| ATOM | 5318 | O | GLY B 289 | 53.005 | -5.326 | 66.358 | 1.00 | 26.17 |
| ATOM | 5319 | N | VAL B 290 | 52.171 | -6.142 | 68.268 | 1.00 | 23.95 |
| ATOM | 5320 | CA | VAL B 290 | 51.194 | -5.079 | 68.440 | 1.00 | 22.25 |
| ATOM | 5321 | CB | VAL B 290 | 49.794 | -5.655 | 68.783 | 1.00 | 18.71 |
| ATOM | 5322 | CG1 | VAL B 290 | 48.810 | -4.525 | 69.047 | 1.00 | 22.67 |
| ATOM | 5323 | CG2 | VAL B 290 | 49.289 | -6.504 | 67.629 | 1.00 | 19.26 |
| ATOM | 5324 | C | VAL B 290 | 51.722 | -4.232 | 69.593 | 1.00 | 21.55 |
| ATOM | 5325 | O | VAL B 290 | 51.960 | -4.741 | 70.687 | 1.00 | 21.32 |
| ATOM | 5326 | N | TYR B 291 | 51.913 | -2.941 | 69.346 | 1.00 | 21.06 |
| ATOM | 5327 | CA | TYR B 291 | 52.479 | -2.063 | 70.357 | 1.00 | 19.29 |
| ATOM | 5328 | CB | TYR B 291 | 53.582 | -1.216 | 69.711 | 1.00 | 20.40 |
| ATOM | 5329 | CG | TYR B 291 | 54.553 | -2.072 | 68.918 | 1.00 | 23.09 |
| ATOM | 5330 | CD1 | TYR B 291 | 54.740 | -1.875 | 67.549 | 1.00 | 19.52 |
| ATOM | 5331 | CE1 | TYR B 291 | 55.580 | -2.712 | 66.809 | 1.00 | 20.67 |
| ATOM | 5332 | CD2 | TYR B 291 | 55.234 | -3.122 | 69.527 | 1.00 | 22.88 |
| ATOM | 5333 | CE2 | TYR B 291 | 56.070 | -3.960 | 68.800 | 1.00 | 26.04 |
| ATOM | 5334 | CZ | TYR B 291 | 56.235 | -3.752 | 67.442 | 1.00 | 23.44 |
| ATOM | 5335 | OH | TYR B 291 | 57.027 | -4.612 | 66.722 | 1.00 | 28.02 |
| ATOM | 5336 | C | TYR B 291 | 51.465 | -1.180 | 71.068 | 1.00 | 26.89 |
| ATOM | 5337 | O | TYR B 291 | 50.668 | -0.479 | 70.429 | 1.00 | 20.26 |
| ATOM | 5338 | N | LEU B 292 | 51.522 | -1.204 | 72.399 | 1.00 | 21.75 |
| ATOM | 5339 | CA | LEU B 292 | 50.604 | -0.426 | 73.227 | 1.00 | 22.11 |
| ATOM | 5340 | CB | LEU B 292 | 49.765 | -1.369 | 74.088 | 1.00 | 20.92 |
| ATOM | 5341 | CG | LEU B 292 | 49.091 | -2.542 | 73.375 | 1.00 | 22.94 |
| ATOM | 5342 | CD1 | LEU B 292 | 48.328 | -3.362 | 74.411 | 1.00 | 21.03 |
| ATOM | 5343 | CD2 | LEU B 292 | 48.149 | -2.043 | 72.281 | 1.00 | 18.04 |
| ATOM | 5344 | C | LEU B 292 | 51.330 | 0.557 | 74.147 | 1.00 | 21.59 |
| ATOM | 5345 | O | LEU B 292 | 52.514 | 0.404 | 74.426 | 1.00 | 19.96 |
| ATOM | 5346 | N | GLY B 293 | 50.606 | 1.571 | 74.613 | 1.00 | 23.31 |
| ATOM | 5347 | CA | GLY B 293 | 51.195 | 2.537 | 75.521 | 1.00 | 20.76 |
| ATOM | 5348 | C | GLY B 293 | 51.163 | 1.979 | 76.930 | 1.00 | 26.15 |
| ATOM | 5349 | O | GLY B 293 | 51.263 | 0.765 | 77.133 | 1.00 | 20.96 |
| ATOM | 5350 | N | GLY B 294 | 51.017 | 2.859 | 77.914 | 1.00 | 24.63 |
| ATOM | 5351 | CA | GLY B 294 | 50.980 | 2.407 | 79.293 | 1.00 | 20.00 |
| ATOM | 5352 | C | GLY B 294 | 51.176 | 3.538 | 80.285 | 1.00 | 22.59 |
| ATOM | 5353 | O | GLY B 294 | 51.145 | 4.719 | 79.916 | 1.00 | 17.46 |
| ATOM | 5354 | N | GLY B 295 | 51.373 | 3.179 | 81.551 | 1.00 | 17.10 |
| ATOM | 5355 | CA | GLY B 295 | 51.577 | 4.180 | 82.582 | 1.00 | 16.52 |
| ATOM | 5356 | C | GLY B 295 | 52.695 | 5.145 | 82.232 | 1.00 | 19.54 |
| ATOM | 5357 | O | GLY B 295 | 53.738 | 4.737 | 81.732 | 1.00 | 16.31 |
| ATOM | 5358 | N | GLY B 296 | 52.467 | 6.430 | 82.497 | 1.00 | 21.93 |
| ATOM | 5359 | CA | GLY B 296 | 53.448 | 7.465 | 82.207 | 1.00 | 20.05 |
| ATOM | 5360 | C | GLY B 296 | 52.869 | 8.750 | 82.759 | 1.00 | 22.20 |
| ATOM | 5361 | O | GLY B 296 | 51.790 | 9.160 | 82.336 | 1.00 | 20.48 |
| ATOM | 5362 | N | TYR B 297 | 53.573 | 9.402 | 83.682 | 1.00 | 20.93 |
| ATOM | 5363 | CA | TYR B 297 | 53.025 | 10.598 | 84.306 | 1.00 | 23.25 |
| ATOM | 5364 | CB | TYR B 297 | 52.731 | 10.284 | 85.774 | 1.00 | 19.93 |
| ATOM | 5365 | CG | TYR B 297 | 52.041 | 8.944 | 85.900 | 1.00 | 24.76 |
| ATOM | 5366 | CD1 | TYR B 297 | 52.779 | 7.758 | 85.936 | 1.00 | 21.97 |
| ATOM | 5367 | CE1 | TYR B 297 | 52.148 | 6.514 | 85.912 | 1.00 | 19.79 |
| ATOM | 5368 | CD2 | TYR B 297 | 50.653 | 8.850 | 85.849 | 1.00 | 20.86 |
| ATOM | 5369 | CE2 | TYR B 297 | 50.012 | 7.612 | 85.822 | 1.00 | 19.57 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-82

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5370 | CZ | TYR | B | 297 | 50.758 | 6.457 | 85.851 | 1.00 | 23.85 |
| ATOM | 5371 | OH | TYR | B | 297 | 50.106 | 5.254 | 85.806 | 1.00 | 17.83 |
| ATOM | 5372 | C | TYR | B | 297 | 53.839 | 11.877 | 84.181 | 1.00 | 25.22 |
| ATOM | 5373 | O | TYR | B | 297 | 53.451 | 12.925 | 84.705 | 1.00 | 21.77 |
| ATOM | 5374 | N | HIS | B | 298 | 54.974 | 11.794 | 83.497 | 1.00 | 23.21 |
| ATOM | 5375 | CA | HIS | B | 298 | 55.787 | 12.976 | 83.270 | 1.00 | 25.62 |
| ATOM | 5376 | CB | HIS | B | 298 | 57.270 | 12.713 | 83.534 | 1.00 | 22.88 |
| ATOM | 5377 | CG | HIS | B | 298 | 58.097 | 13.956 | 83.502 | 1.00 | 25.13 |
| ATOM | 5378 | CD2 | HIS | B | 298 | 58.406 | 14.791 | 82.482 | 1.00 | 28.22 |
| ATOM | 5379 | ND1 | HIS | B | 298 | 58.617 | 14.536 | 84.641 | 1.00 | 32.76 |
| ATOM | 5380 | CE1 | HIS | B | 298 | 59.209 | 15.674 | 84.323 | 1.00 | 26.52 |
| ATOM | 5381 | NE2 | HIS | B | 298 | 59.094 | 15.852 | 83.019 | 1.00 | 32.15 |
| ATOM | 5382 | C | HIS | B | 298 | 55.589 | 13.307 | 81.795 | 1.00 | 25.66 |
| ATOM | 5383 | O | HIS | B | 298 | 56.087 | 12.589 | 80.923 | 1.00 | 25.84 |
| ATOM | 5384 | N | PRO | B | 299 | 54.901 | 14.424 | 81.496 | 1.00 | 27.02 |
| ATOM | 5385 | CD | PRO | B | 299 | 54.388 | 15.424 | 82.447 | 1.00 | 29.91 |
| ATOM | 5386 | CA | PRO | B | 299 | 54.616 | 14.864 | 80.127 | 1.00 | 26.53 |
| ATOM | 5387 | CB | PRO | B | 299 | 53.952 | 16.232 | 80.342 | 1.00 | 27.76 |
| ATOM | 5388 | CG | PRO | B | 299 | 54.583 | 16.696 | 81.656 | 1.00 | 27.97 |
| ATOM | 5389 | C | PRO | B | 299 | 55.815 | 14.930 | 79.194 | 1.00 | 27.08 |
| ATOM | 5390 | O | PRO | B | 299 | 55.738 | 14.472 | 78.057 | 1.00 | 28.58 |
| ATOM | 5391 | N | TYR | B | 300 | 56.925 | 15.484 | 79.668 | 1.00 | 27.30 |
| ATOM | 5392 | CA | TYR | B | 300 | 58.114 | 15.593 | 78.824 | 1.00 | 27.17 |
| ATOM | 5393 | CB | TYR | B | 300 | 59.173 | 16.496 | 79.466 | 1.00 | 31.65 |
| ATOM | 5394 | CG | TYR | B | 300 | 58.684 | 17.851 | 79.921 | 1.00 | 31.61 |
| ATOM | 5395 | CD1 | TYR | B | 300 | 57.414 | 18.318 | 79.582 | 1.00 | 32.71 |
| ATOM | 5396 | CE1 | TYR | B | 300 | 56.971 | 19.568 | 80.014 | 1.00 | 38.52 |
| ATOM | 5397 | CD2 | TYR | B | 300 | 59.499 | 18.670 | 80.701 | 1.00 | 30.92 |
| ATOM | 5398 | CE2 | TYR | B | 300 | 59.072 | 19.917 | 81.138 | 1.00 | 32.13 |
| ATOM | 5399 | CZ | TYR | B | 300 | 57.808 | 20.361 | 80.795 | 1.00 | 39.17 |
| ATOM | 5400 | OH | TYR | B | 300 | 57.374 | 21.585 | 81.252 | 1.00 | 43.90 |
| ATOM | 5401 | C | TYR | B | 300 | 58.731 | 14.218 | 78.572 | 1.00 | 25.20 |
| ATOM | 5402 | O | TYR | B | 300 | 59.106 | 13.894 | 77.445 | 1.00 | 25.15 |
| ATOM | 5403 | N | ALA | B | 301 | 58.845 | 13.419 | 79.628 | 1.00 | 20.55 |
| ATOM | 5404 | CA | ALA | B | 301 | 59.414 | 12.080 | 79.508 | 1.00 | 22.12 |
| ATOM | 5405 | CB | ALA | B | 301 | 59.417 | 11.388 | 80.874 | 1.00 | 17.09 |
| ATOM | 5406 | C | ALA | B | 301 | 58.608 | 11.260 | 78.505 | 1.00 | 15.20 |
| ATOM | 5407 | O | ALA | B | 301 | 59.161 | 10.629 | 77.613 | 1.00 | 17.12 |
| ATOM | 5408 | N | LEU | B | 302 | 57.295 | 11.290 | 78.667 | 1.00 | 18.02 |
| ATOM | 5409 | CA | LEU | B | 302 | 56.381 | 10.553 | 77.815 | 1.00 | 19.88 |
| ATOM | 5410 | CB | LEU | B | 302 | 54.957 | 10.702 | 78.362 | 1.00 | 21.72 |
| ATOM | 5411 | CG | LEU | B | 302 | 53.767 | 10.118 | 77.606 | 1.00 | 31.08 |
| ATOM | 5412 | CD1 | LEU | B | 302 | 52.576 | 9.980 | 78.549 | 1.00 | 31.35 |
| ATOM | 5413 | CD2 | LEU | B | 302 | 53.434 | 11.011 | 76.415 | 1.00 | 27.11 |
| ATOM | 5414 | C | LEU | B | 302 | 56.445 | 10.988 | 76.351 | 1.00 | 21.13 |
| ATOM | 5415 | O | LEU | B | 302 | 56.473 | 10.149 | 75.449 | 1.00 | 21.76 |
| ATOM | 5416 | N | ALA | B | 303 | 56.472 | 12.293 | 76.115 | 1.00 | 17.69 |
| ATOM | 5417 | CA | ALA | B | 303 | 56.516 | 12.811 | 74.755 | 1.00 | 17.79 |
| ATOM | 5418 | CB | ALA | B | 303 | 56.357 | 14.326 | 74.780 | 1.00 | 24.50 |
| ATOM | 5419 | C | ALA | B | 303 | 57.803 | 12.425 | 74.040 | 1.00 | 20.84 |
| ATOM | 5420 | O | ALA | B | 303 | 57.781 | 11.968 | 72.891 | 1.00 | 19.33 |
| ATOM | 5421 | N | ARG | B | 304 | 58.930 | 12.594 | 74.723 | 1.00 | 21.08 |
| ATOM | 5422 | CA | ARG | B | 304 | 60.215 | 12.269 | 74.120 | 1.00 | 25.56 |
| ATOM | 5423 | CB | ARG | B | 304 | 61.375 | 12.825 | 74.962 | 1.00 | 18.37 |
| ATOM | 5424 | CG | ARG | B | 304 | 61.427 | 14.356 | 75.072 | 1.00 | 23.12 |
| ATOM | 5425 | CD | ARG | B | 304 | 62.797 | 14.758 | 75.624 | 1.00 | 29.00 |
| ATOM | 5426 | NE | ARG | B | 304 | 63.073 | 13.938 | 76.789 | 1.00 | 33.28 |
| ATOM | 5427 | CZ | ARG | B | 304 | 64.271 | 13.689 | 77.283 | 1.00 | 30.24 |
| ATOM | 5428 | NH1 | ARG | B | 304 | 65.363 | 14.194 | 76.723 | 1.00 | 24.98 |
| ATOM | 5429 | NH2 | ARG | B | 304 | 64.365 | 12.896 | 78.333 | 1.00 | 36.15 |
| ATOM | 5430 | C | ARG | B | 304 | 60.406 | 10.775 | 73.922 | 1.00 | 20.46 |
| ATOM | 5431 | O | ARG | B | 304 | 60.850 | 10.338 | 72.868 | 1.00 | 18.70 |
| ATOM | 5432 | N | ALA | B | 305 | 60.070 | 9.988 | 74.937 | 1.00 | 22.48 |
| ATOM | 5433 | CA | ALA | B | 305 | 60.226 | 8.542 | 74.845 | 1.00 | 19.70 |
| ATOM | 5434 | CB | ALA | B | 305 | 59.847 | 7.894 | 76.174 | 1.00 | 24.24 |
| ATOM | 5435 | C | ALA | B | 305 | 59.407 | 7.930 | 73.711 | 1.00 | 15.82 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-83

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5436 | O | ALA | B | 305 | 59.938 | 7.184 | 72.888 | 1.00 | 19.12 |
| ATOM | 5437 | N | TRP | B | 306 | 58.113 | 8.230 | 73.659 | 1.00 | 18.65 |
| ATOM | 5438 | CA | TRP | B | 306 | 57.298 | 7.668 | 72.600 | 1.00 | 19.57 |
| ATOM | 5439 | CB | TRP | B | 306 | 55.800 | 7.856 | 72.893 | 1.00 | 18.26 |
| ATOM | 5440 | CG | TRP | B | 306 | 55.301 | 6.911 | 73.953 | 1.00 | 20.71 |
| ATOM | 5441 | CD2 | TRP | B | 306 | 54.087 | 7.025 | 74.708 | 1.00 | 23.94 |
| ATOM | 5442 | CE2 | TRP | B | 306 | 53.988 | 5.870 | 75.513 | 1.00 | 24.73 |
| ATOM | 5443 | CE3 | TRP | B | 306 | 53.073 | 7.991 | 74.780 | 1.00 | 26.01 |
| ATOM | 5444 | CD1 | TRP | B | 306 | 55.872 | 5.721 | 74.326 | 1.00 | 20.04 |
| ATOM | 5445 | NE1 | TRP | B | 306 | 55.092 | 5.093 | 75.260 | 1.00 | 19.17 |
| ATOM | 5446 | CZ2 | TRP | B | 306 | 52.912 | 5.655 | 76.385 | 1.00 | 28.04 |
| ATOM | 5447 | CZ3 | TRP | B | 306 | 52.001 | 7.779 | 75.646 | 1.00 | 28.68 |
| ATOM | 5448 | CH2 | TRP | B | 306 | 51.930 | 6.619 | 76.437 | 1.00 | 31.22 |
| ATOM | 5449 | C | TRP | B | 306 | 57.665 | 8.223 | 71.226 | 1.00 | 23.48 |
| ATOM | 5450 | O | TRP | B | 306 | 57.416 | 7.574 | 70.212 | 1.00 | 22.38 |
| ATOM | 5451 | N | THR | B | 307 | 58.262 | 9.412 | 71.176 | 1.00 | 22.36 |
| ATOM | 5452 | CA | THR | B | 307 | 58.672 | 9.953 | 69.880 | 1.00 | 25.94 |
| ATOM | 5453 | CB | THR | B | 307 | 59.143 | 11.417 | 69.986 | 1.00 | 25.88 |
| ATOM | 5454 | OG1 | THR | B | 307 | 58.015 | 12.261 | 70.258 | 1.00 | 21.07 |
| ATOM | 5455 | CG2 | THR | B | 307 | 59.827 | 11.864 | 68.686 | 1.00 | 22.52 |
| ATOM | 5456 | C | THR | B | 307 | 59.815 | 9.078 | 69.350 | 1.00 | 30.09 |
| ATOM | 5457 | O | THR | B | 307 | 59.922 | 8.834 | 68.144 | 1.00 | 25.82 |
| ATOM | 5458 | N | LEU | B | 308 | 60.664 | 8.596 | 70.258 | 1.00 | 27.54 |
| ATOM | 5459 | CA | LEU | B | 308 | 61.773 | 7.734 | 69.857 | 1.00 | 26.76 |
| ATOM | 5460 | CB | LEU | B | 308 | 62.691 | 7.424 | 71.054 | 1.00 | 24.24 |
| ATOM | 5461 | CG | LEU | B | 308 | 63.420 | 8.614 | 71.718 | 1.00 | 31.16 |
| ATOM | 5462 | CD1 | LEU | B | 308 | 64.282 | 8.147 | 72.877 | 1.00 | 24.71 |
| ATOM | 5463 | CD2 | LEU | B | 308 | 64.289 | 9.325 | 70.700 | 1.00 | 24.59 |
| ATOM | 5464 | C | LEU | B | 308 | 61.184 | 6.443 | 69.287 | 1.00 | 27.20 |
| ATOM | 5465 | O | LEU | B | 308 | 61.609 | 5.961 | 68.234 | 1.00 | 23.52 |
| ATOM | 5466 | N | ILE | B | 309 | 60.190 | 5.898 | 69.980 | 1.00 | 25.10 |
| ATOM | 5467 | CA | ILE | B | 309 | 59.537 | 4.679 | 69.530 | 1.00 | 25.14 |
| ATOM | 5468 | CB | ILE | B | 309 | 58.387 | 4.266 | 70.485 | 1.00 | 27.05 |
| ATOM | 5469 | CG2 | ILE | B | 309 | 57.646 | 3.058 | 69.926 | 1.00 | 23.57 |
| ATOM | 5470 | CG1 | ILE | B | 309 | 58.952 | 3.947 | 71.868 | 1.00 | 22.98 |
| ATOM | 5471 | CD1 | ILE | B | 309 | 59.927 | 2.793 | 71.868 | 1.00 | 24.25 |
| ATOM | 5472 | C | ILE | B | 309 | 58.958 | 4.885 | 68.133 | 1.00 | 25.41 |
| ATOM | 5473 | O | ILE | B | 309 | 59.177 | 4.064 | 67.243 | 1.00 | 22.13 |
| ATOM | 5474 | N | TRP | B | 310 | 58.232 | 5.984 | 67.943 | 1.00 | 27.45 |
| ATOM | 5475 | CA | TRP | B | 310 | 57.618 | 6.266 | 66.648 | 1.00 | 29.27 |
| ATOM | 5476 | CB | TRP | B | 310 | 56.721 | 7.505 | 66.715 | 1.00 | 27.00 |
| ATOM | 5477 | CG | TRP | B | 310 | 56.112 | 7.847 | 65.378 | 1.00 | 28.26 |
| ATOM | 5478 | CD2 | TRP | B | 310 | 55.172 | 7.061 | 64.633 | 1.00 | 27.50 |
| ATOM | 5479 | CE2 | TRP | B | 310 | 54.947 | 7.729 | 63.408 | 1.00 | 30.47 |
| ATOM | 5480 | CE3 | TRP | B | 310 | 54.500 | 5.856 | 64.877 | 1.00 | 29.85 |
| ATOM | 5481 | CD1 | TRP | B | 310 | 56.406 | 8.929 | 64.597 | 1.00 | 29.76 |
| ATOM | 5482 | NE1 | TRP | B | 310 | 55.713 | 8.865 | 63.415 | 1.00 | 26.71 |
| ATOM | 5483 | CZ2 | TRP | B | 310 | 54.076 | 8.234 | 62.429 | 1.00 | 28.23 |
| ATOM | 5484 | CZ3 | TRP | B | 310 | 53.636 | 5.362 | 63.901 | 1.00 | 30.24 |
| ATOM | 5485 | CH2 | TRP | B | 310 | 53.433 | 6.053 | 62.692 | 1.00 | 27.63 |
| ATOM | 5486 | C | TRP | B | 310 | 58.629 | 6.424 | 65.520 | 1.00 | 30.16 |
| ATOM | 5487 | O | TRP | B | 310 | 58.378 | 5.964 | 64.410 | 1.00 | 30.04 |
| ATOM | 5488 | N | CYS | B | 311 | 59.762 | 7.069 | 65.793 | 1.00 | 24.26 |
| ATOM | 5489 | CA | CYS | B | 311 | 60.782 | 7.233 | 64.764 | 1.00 | 27.97 |
| ATOM | 5490 | CB | CYS | B | 311 | 61.893 | 8.157 | 65.252 | 1.00 | 28.21 |
| ATOM | 5491 | SG | CYS | B | 311 | 61.422 | 9.905 | 65.381 | 1.00 | 33.38 |
| ATOM | 5492 | C | CYS | B | 311 | 61.380 | 5.886 | 64.351 | 1.00 | 30.02 |
| ATOM | 5493 | O | CYS | B | 311 | 61.670 | 5.660 | 63.172 | 1.00 | 25.45 |
| ATOM | 5494 | N | GLU | B | 312 | 61.570 | 5.001 | 65.327 | 1.00 | 31.59 |
| ATOM | 5495 | CA | GLU | B | 312 | 62.111 | 3.669 | 65.067 | 1.00 | 33.48 |
| ATOM | 5496 | CB | GLU | B | 312 | 62.142 | 2.843 | 66.352 | 1.00 | 34.78 |
| ATOM | 5497 | CG | GLU | B | 312 | 63.487 | 2.307 | 66.758 | 1.00 | 39.45 |
| ATOM | 5498 | CD | GLU | B | 312 | 64.171 | 1.513 | 65.675 | 1.00 | 40.11 |
| ATOM | 5499 | OE1 | GLU | B | 312 | 63.539 | 0.614 | 65.081 | 1.00 | 43.69 |
| ATOM | 5500 | OE2 | GLU | B | 312 | 65.358 | 1.782 | 65.437 | 1.00 | 39.26 |
| ATOM | 5501 | C | GLU | B | 312 | 61.197 | 2.959 | 64.080 | 1.00 | 29.97 |

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Figure 18-84.

| | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 5502 | O | GLU B 312 | 61.640 | 2.497 | 63.035 | 1.00 | 31.38 |
| ATOM | 5503 | N | LEU B 313 | 59.919 | 2.865 | 64.438 | 1.00 | 26.70 |
| ATOM | 5504 | CA | LEU B 313 | 58.930 | 2.203 | 63.598 | 1.00 | 26.73 |
| ATOM | 5505 | CB | LEU B 313 | 57.571 | 2.173 | 64.297 | 1.00 | 25.83 |
| ATOM | 5506 | CG | LEU B 313 | 57.429 | 1.224 | 65.477 | 1.00 | 35.18 |
| ATOM | 5507 | CD1 | LEU B 313 | 56.063 | 1.434 | 66.130 | 1.00 | 32.49 |
| ATOM | 5508 | CD2 | LEU B 313 | 57.595 | -0.215 | 64.989 | 1.00 | 29.71 |
| ATOM | 5509 | C | LEU B 313 | 58.768 | 2.866 | 62.248 | 1.00 | 29.03 |
| ATOM | 5510 | O | LEU B 313 | 58.716 | 2.187 | 61.228 | 1.00 | 25.39 |
| ATOM | 5511 | N | SER B 314 | 58.677 | 4.194 | 62.263 | 1.00 | 30.13 |
| ATOM | 5512 | CA | SER B 314 | 58.498 | 5.006 | 61.060 | 1.00 | 34.06 |
| ATOM | 5513 | CB | SER B 314 | 58.206 | 6.456 | 61.445 | 1.00 | 31.15 |
| ATOM | 5514 | OG | SER B 314 | 57.041 | 6.537 | 62.234 | 1.00 | 48.58 |
| ATOM | 5515 | C | SER B 314 | 59.707 | 5.003 | 60.151 | 1.00 | 31.84 |
| ATOM | 5516 | O | SER B 314 | 59.632 | 5.469 | 59.026 | 1.00 | 34.15 |
| ATOM | 5517 | N | GLY B 315 | 60.831 | 4.515 | 60.655 | 1.00 | 31.81 |
| ATOM | 5518 | CA | GLY B 315 | 62.036 | 4.485 | 59.848 | 1.00 | 37.27 |
| ATOM | 5519 | C | GLY B 315 | 62.659 | 5.851 | 59.616 | 1.00 | 39.93 |
| ATOM | 5520 | O | GLY B 315 | 63.363 | 6.054 | 58.624 | 1.00 | 39.79 |
| ATOM | 5521 | N | ARG B 316 | 62.422 | 6.798 | 60.518 | 1.00 | 38.22 |
| ATOM | 5522 | CA | ARG B 316 | 63.004 | 8.121 | 60.336 | 1.00 | 38.66 |
| ATOM | 5523 | CB | ARG B 316 | 61.908 | 9.184 | 60.275 | 1.00 | 40.20 |
| ATOM | 5524 | CG | ARG B 316 | 61.089 | 9.345 | 61.520 | 1.00 | 39.00 |
| ATOM | 5525 | CD | ARG B 316 | 60.032 | 10.398 | 61.284 | 1.00 | 42.13 |
| ATOM | 5526 | NE | ARG B 316 | 59.002 | 9.954 | 60.352 | 1.00 | 45.09 |
| ATOM | 5527 | CZ | ARG B 316 | 58.075 | 10.754 | 59.838 | 1.00 | 40.84 |
| ATOM | 5528 | NH1 | ARG B 316 | 58.064 | 12.033 | 60.170 | 1.00 | 48.44 |
| ATOM | 5529 | NH2 | ARG B 316 | 57.150 | 10.278 | 59.014 | 1.00 | 35.96 |
| ATOM | 5530 | C | ARG B 316 | 64.031 | 8.467 | 61.408 | 1.00 | 39.03 |
| ATOM | 5531 | O | ARG B 316 | 63.952 | 7.988 | 62.539 | 1.00 | 34.34 |
| ATOM | 5532 | N | GLU B 317 | 65.003 | 9.296 | 61.035 | 1.00 | 39.58 |
| ATOM | 5533 | CA | GLU B 317 | 66.074 | 9.697 | 61.943 | 1.00 | 43.35 |
| ATOM | 5534 | CB | GLU B 317 | 67.142 | 10.509 | 61.203 | 1.00 | 49.34 |
| ATOM | 5535 | CG | GLU B 317 | 67.609 | 9.910 | 59.884 | 1.00 | 57.04 |
| ATOM | 5536 | CD | GLU B 317 | 66.546 | 10.009 | 58.798 | 1.00 | 62.79 |
| ATOM | 5537 | OE1 | GLU B 317 | 66.146 | 11.149 | 58.467 | 1.00 | 63.46 |
| ATOM | 5538 | OE2 | GLU B 317 | 66.108 | 8.954 | 58.280 | 1.00 | 64.46 |
| ATOM | 5539 | C | GLU B 317 | 65.555 | 10.528 | 63.100 | 1.00 | 41.58 |
| ATOM | 5540 | O | GLU B 317 | 64.658 | 11.356 | 62.939 | 1.00 | 39.74 |
| ATOM | 5541 | N | VAL B 318 | 66.118 | 10.301 | 64.278 | 1.00 | 35.38 |
| ATOM | 5542 | CA | VAL B 318 | 65.706 | 11.049 | 65.448 | 1.00 | 38.76 |
| ATOM | 5543 | CB | VAL B 318 | 66.000 | 10.265 | 66.750 | 1.00 | 42.28 |
| ATOM | 5544 | CG1 | VAL B 318 | 65.560 | 11.080 | 67.962 | 1.00 | 38.26 |
| ATOM | 5545 | CG2 | VAL B 318 | 65.287 | 8.916 | 66.722 | 1.00 | 39.99 |
| ATOM | 5546 | C | VAL B 318 | 66.459 | 12.370 | 65.478 | 1.00 | 41.82 |
| ATOM | 5547 | O | VAL B 318 | 67.689 | 12.395 | 65.570 | 1.00 | 37.20 |
| ATOM | 5548 | N | PRO B 319 | 65.735 | 13.491 | 65.356 | 1.00 | 43.18 |
| ATOM | 5549 | CD | PRO B 319 | 64.290 | 13.672 | 65.155 | 1.00 | 41.90 |
| ATOM | 5550 | CA | PRO B 319 | 66.402 | 14.792 | 65.388 | 1.00 | 44.31 |
| ATOM | 5551 | CB | PRO B 319 | 65.241 | 15.763 | 65.181 | 1.00 | 44.58 |
| ATOM | 5552 | CG | PRO B 319 | 64.079 | 15.011 | 65.795 | 1.00 | 43.34 |
| ATOM | 5553 | C | PRO B 319 | 67.086 | 14.965 | 66.741 | 1.00 | 44.62 |
| ATOM | 5554 | O | PRO B 319 | 66.541 | 14.565 | 67.771 | 1.00 | 43.75 |
| ATOM | 5555 | N | GLU B 320 | 68.277 | 15.552 | 66.735 | 1.00 | 44.16 |
| ATOM | 5556 | CA | GLU B 320 | 69.029 | 15.762 | 67.967 | 1.00 | 45.92 |
| ATOM | 5557 | CB | GLU B 320 | 70.381 | 16.406 | 67.663 | 1.00 | 50.87 |
| ATOM | 5558 | CG | GLU B 320 | 71.165 | 16.768 | 68.919 | 1.00 | 53.71 |
| ATOM | 5559 | CD | GLU B 320 | 72.455 | 17.505 | 68.620 | 1.00 | 57.75 |
| ATOM | 5560 | OE1 | GLU B 320 | 73.161 | 17.874 | 69.583 | 1.00 | 56.37 |
| ATOM | 5561 | OE2 | GLU B 320 | 72.762 | 17.714 | 67.427 | 1.00 | 60.07 |
| ATOM | 5562 | C | GLU B 320 | 68.311 | 16.625 | 68.995 | 1.00 | 44.42 |
| ATOM | 5563 | O | GLU B 320 | 68.244 | 16.279 | 70.168 | 1.00 | 42.32 |
| ATOM | 5564 | N | LYS B 321 | 67.778 | 17.753 | 68.550 | 1.00 | 42.50 |
| ATOM | 5565 | CA | LYS B 321 | 67.102 | 18.672 | 69.448 | 1.00 | 45.24 |
| ATOM | 5566 | CB | LYS B 321 | 67.853 | 20.000 | 69.503 | 1.00 | 46.43 |
| ATOM | 5567 | CG | LYS B 321 | 67.890 | 20.802 | 68.195 | 1.00 | 51.45 |

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Figure 18-85

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5568 | CD | LYS | B | 321 | 68.700 | 20.144 | 67.057 | 1.00 | 57.24 |
| ATOM | 5569 | CE | LYS | B | 321 | 67.936 | 19.062 | 66.280 | 1.00 | 55.24 |
| ATOM | 5570 | NZ | LYS | B | 321 | 66.738 | 19.588 | 65.558 | 1.00 | 55.31 |
| ATOM | 5571 | C | LYS | B | 321 | 65.662 | 18.971 | 69.098 | 1.00 | 43.44 |
| ATOM | 5572 | O | LYS | B | 321 | 65.211 | 18.736 | 67.978 | 1.00 | 43.03 |
| ATOM | 5573 | N | LEU | B | 322 | 64.947 | 19.512 | 70.076 | 1.00 | 39.45 |
| ATOM | 5574 | CA | LEU | B | 322 | 63.563 | 19.885 | 69.875 | 1.00 | 40.31 |
| ATOM | 5575 | CB | LEU | B | 322 | 62.846 | 20.034 | 71.215 | 1.00 | 40.88 |
| ATOM | 5576 | CG | LEU | B | 322 | 62.943 | 18.901 | 72.234 | 1.00 | 40.09 |
| ATOM | 5577 | CD1 | LEU | B | 322 | 62.001 | 19.175 | 73.388 | 1.00 | 38.17 |
| ATOM | 5578 | CD2 | LEU | B | 322 | 62.588 | 17.596 | 71.580 | 1.00 | 41.56 |
| ATOM | 5579 | C | LEU | B | 322 | 63.615 | 21.244 | 59.197 | 1.00 | 41.23 |
| ATOM | 5580 | O | LEU | B | 322 | 64.466 | 22.070 | 69.531 | 1.00 | 39.22 |
| ATOM | 5581 | N | ASN | B | 323 | 62.735 | 21.473 | 68.233 | 1.00 | 40.04 |
| ATOM | 5582 | CA | ASN | B | 323 | 62.703 | 22.771 | 67.582 | 1.00 | 43.32 |
| ATOM | 5583 | CB | ASN | B | 323 | 61.985 | 22.707 | 66.234 | 1.00 | 41.53 |
| ATOM | 5584 | CG | ASN | B | 323 | 60.617 | 22.085 | 66.335 | 1.00 | 41.89 |
| ATOM | 5585 | OD1 | ASN | B | 323 | 59.889 | 22.308 | 67.304 | 1.00 | 39.79 |
| ATOM | 5586 | ND2 | ASN | B | 323 | 60.243 | 21.317 | 65.317 | 1.00 | 40.43 |
| ATOM | 5587 | C | ASN | B | 323 | 61.949 | 23.690 | 68.532 | 1.00 | 44.76 |
| ATOM | 5588 | O | ASN | B | 323 | 61.402 | 23.237 | 69.539 | 1.00 | 45.80 |
| ATOM | 5589 | N | ASN | B | 324 | 61.902 | 24.973 | 68.210 | 1.00 | 46.85 |
| ATOM | 5590 | CA | ASN | B | 324 | 61.234 | 25.930 | 69.076 | 1.00 | 47.60 |
| ATOM | 5591 | CB | ASN | B | 324 | 61.460 | 27.348 | 68.549 | 1.00 | 50.87 |
| ATOM | 5592 | CG | ASN | B | 324 | 61.089 | 28.407 | 69.562 | 1.00 | 55.06 |
| ATOM | 5593 | OD1 | ASN | B | 324 | 59.925 | 28.565 | 69.919 | 1.00 | 60.68 |
| ATOM | 5594 | ND2 | ASN | B | 324 | 62.091 | 29.131 | 70.048 | 1.00 | 59.17 |
| ATOM | 5595 | C | ASN | B | 324 | 59.740 | 25.664 | 69.249 | 1.00 | 43.97 |
| ATOM | 5596 | O | ASN | B | 324 | 59.190 | 25.898 | 70.322 | 1.00 | 41.33 |
| ATOM | 5597 | N | LYS | B | 325 | 59.087 | 25.168 | 68.201 | 1.00 | 43.49 |
| ATOM | 5598 | CA | LYS | B | 325 | 57.655 | 24.892 | 68.264 | 1.00 | 45.95 |
| ATOM | 5599 | CB | LYS | B | 325 | 57.112 | 24.415 | 66.909 | 1.00 | 48.97 |
| ATOM | 5600 | CG | LYS | B | 325 | 57.212 | 25.400 | 65.731 | 1.00 | 53.41 |
| ATOM | 5601 | CD | LYS | B | 325 | 58.582 | 25.386 | 65.024 | 1.00 | 58.77 |
| ATOM | 5602 | CE | LYS | B | 325 | 59.700 | 26.013 | 65.846 | 1.00 | 58.10 |
| ATOM | 5603 | NZ | LYS | B | 325 | 61.024 | 25.906 | 65.178 | 1.00 | 53.38 |
| ATOM | 5604 | C | LYS | B | 325 | 57.368 | 23.822 | 69.309 | 1.00 | 45.79 |
| ATOM | 5605 | O | LYS | B | 325 | 56.375 | 23.891 | 70.034 | 1.00 | 43.91 |
| ATOM | 5606 | N | ALA | B | 326 | 58.245 | 22.829 | 69.381 | 1.00 | 44.28 |
| ATOM | 5607 | CA | ALA | B | 326 | 58.078 | 21.746 | 70.336 | 1.00 | 44.25 |
| ATOM | 5608 | CB | ALA | B | 326 | 59.013 | 20.589 | 69.986 | 1.00 | 41.44 |
| ATOM | 5609 | C | ALA | B | 326 | 58.342 | 22.233 | 71.757 | 1.00 | 40.92 |
| ATOM | 5610 | O | ALA | B | 326 | 57.639 | 21.843 | 72.688 | 1.00 | 39.02 |
| ATOM | 5611 | N | LYS | B | 327 | 59.352 | 23.085 | 71.922 | 1.00 | 38.14 |
| ATOM | 5612 | CA | LYS | B | 327 | 59.689 | 23.603 | 73.246 | 1.00 | 40.11 |
| ATOM | 5613 | CB | LYS | B | 327 | 60.892 | 24.552 | 73.178 | 1.00 | 42.36 |
| ATOM | 5614 | CG | LYS | B | 327 | 62.174 | 23.922 | 72.159 | 1.00 | 45.78 |
| ATOM | 5615 | CD | LYS | B | 327 | 63.325 | 24.926 | 72.675 | 1.00 | 48.46 |
| ATOM | 5616 | CE | LYS | B | 327 | 64.594 | 24.367 | 72.031 | 1.00 | 49.62 |
| ATOM | 5617 | NZ | LYS | B | 327 | 65.108 | 23.139 | 72.700 | 1.00 | 48.53 |
| ATOM | 5618 | C | LYS | B | 327 | 58.500 | 24.338 | 73.841 | 1.00 | 39.17 |
| ATOM | 5619 | O | LYS | B | 327 | 58.132 | 24.112 | 74.994 | 1.00 | 38.87 |
| ATOM | 5620 | N | GLU | B | 328 | 57.898 | 25.215 | 73.048 | 1.00 | 41.06 |
| ATOM | 5621 | CA | GLU | B | 328 | 56.750 | 25.986 | 73.512 | 1.00 | 42.35 |
| ATOM | 5622 | CB | GLU | B | 328 | 56.357 | 27.028 | 72.463 | 1.00 | 44.02 |
| ATOM | 5623 | CG | GLU | B | 328 | 57.434 | 28.084 | 72.258 | 1.00 | 44.80 |
| ATOM | 5624 | CD | GLU | B | 328 | 57.835 | 28.742 | 73.569 | 1.00 | 48.40 |
| ATOM | 5625 | OE1 | GLU | B | 328 | 56.949 | 29.317 | 74.237 | 1.00 | 51.20 |
| ATOM | 5626 | OE2 | GLU | B | 328 | 59.029 | 28.680 | 73.935 | 1.00 | 47.81 |
| ATOM | 5627 | C | GLU | B | 328 | 55.569 | 25.087 | 73.839 | 1.00 | 38.67 |
| ATOM | 5628 | O | GLU | B | 328 | 54.794 | 25.377 | 74.750 | 1.00 | 41.20 |
| ATOM | 5629 | N | LEU | B | 329 | 55.429 | 23.999 | 73.090 | 1.00 | 35.31 |
| ATOM | 5630 | CA | LEU | B | 329 | 54.349 | 23.056 | 73.334 | 1.00 | 32.69 |
| ATOM | 5631 | CB | LEU | B | 329 | 54.404 | 21.900 | 72.334 | 1.00 | 35.06 |
| ATOM | 5632 | CG | LEU | B | 329 | 53.344 | 20.813 | 72.544 | 1.00 | 35.01 |
| ATOM | 5633 | CD1 | LEU | B | 329 | 51.958 | 21.430 | 72.419 | 1.00 | 36.90 |

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Figure 18-86

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5634 | CD2 | LEU | B | 329 | 53.521 | 19.699 | 71.525 | 1.00 | 32.36 |
| ATOM | 5635 | C | LEU | B | 329 | 54.504 | 22.507 | 74.747 | 1.00 | 34.07 |
| ATOM | 5636 | O | LEU | B | 329 | 53.621 | 22.664 | 75.583 | 1.00 | 30.53 |
| ATOM | 5637 | N | LEU | B | 330 | 55.640 | 21.873 | 75.013 | 1.00 | 32.74 |
| ATOM | 5638 | CA | LEU | B | 330 | 55.889 | 21.311 | 76.330 | 1.00 | 34.99 |
| ATOM | 5639 | CB | LEU | B | 330 | 57.267 | 20.642 | 76.382 | 1.00 | 37.01 |
| ATOM | 5640 | CG | LEU | B | 330 | 57.466 | 19.428 | 75.470 | 1.00 | 34.91 |
| ATOM | 5641 | CD1 | LEU | B | 330 | 58.832 | 18.817 | 75.728 | 1.00 | 34.69 |
| ATOM | 5642 | CD2 | LEU | B | 330 | 56.369 | 18.396 | 75.742 | 1.00 | 34.10 |
| ATOM | 5643 | C | LEU | B | 330 | 55.789 | 22.363 | 77.429 | 1.00 | 37.12 |
| ATOM | 5644 | Q | LEU | B | 330 | 55.210 | 22.110 | 78.482 | 1.00 | 34.19 |
| ATOM | 5645 | N | LYS | B | 331 | 56.353 | 23.540 | 77.186 | 1.00 | 34.34 |
| ATOM | 5646 | CA | LYS | B | 331 | 56.313 | 24.604 | 78.181 | 1.00 | 43.35 |
| ATOM | 5647 | CB | LYS | B | 331 | 57.162 | 25.788 | 77.712 | 1.00 | 46.25 |
| ATOM | 5648 | CG | LYS | B | 331 | 58.658 | 25.496 | 77.685 | 1.00 | 51.07 |
| ATOM | 5649 | CD | LYS | B | 331 | 59.482 | 26.610 | 77.021 | 1.00 | 49.96 |
| ATOM | 5650 | CE | LYS | B | 331 | 59.371 | 27.957 | 77.733 | 1.00 | 53.08 |
| ATOM | 5651 | NZ | LYS | B | 331 | 58.013 | 28.569 | 77.662 | 1.00 | 56.18 |
| ATOM | 5652 | C | LYS | B | 331 | 54.892 | 25.069 | 78.494 | 1.00 | 42.06 |
| ATOM | 5653 | O | LYS | B | 331 | 54.588 | 25.416 | 79.631 | 1.00 | 43.05 |
| ATOM | 5654 | N | SER | B | 332 | 54.018 | 25.056 | 77.492 | 1.00 | 44.54 |
| ATOM | 5655 | CA | SER | B | 332 | 52.639 | 25.502 | 77.679 | 1.00 | 46.58 |
| ATOM | 5656 | CB | SER | B | 332 | 51.975 | 25.751 | 76.329 | 1.00 | 48.75 |
| ATOM | 5657 | OG | SER | B | 332 | 51.769 | 24.527 | 75.646 | 1.00 | 49.55 |
| ATOM | 5658 | C | SER | B | 332 | 51.780 | 24.507 | 78.451 | 1.00 | 49.56 |
| ATOM | 5659 | O | SER | B | 332 | 50.618 | 24.791 | 78.749 | 1.00 | 46.67 |
| ATOM | 5660 | N | ILE | B | 333 | 52.341 | 23.345 | 78.770 | 1.00 | 50.55 |
| ATOM | 5661 | CA | ILE | B | 333 | 51.586 | 22.326 | 79.488 | 1.00 | 51.93 |
| ATOM | 5662 | CB | ILE | B | 333 | 52.259 | 20.945 | 79.376 | 1.00 | 51.82 |
| ATOM | 5663 | CG2 | ILE | B | 333 | 51.447 | 19.902 | 80.134 | 1.00 | 50.29 |
| ATOM | 5664 | CG1 | ILE | B | 333 | 52.359 | 20.539 | 77.905 | 1.00 | 52.18 |
| ATOM | 5665 | CD1 | ILE | B | 333 | 53.044 | 19.210 | 77.693 | 1.00 | 55.42 |
| ATOM | 5666 | C | ILE | B | 333 | 51.367 | 22.634 | 80.964 | 1.00 | 51.45 |
| ATOM | 5667 | O | ILE | B | 333 | 52.180 | 23.290 | 81.614 | 1.00 | 50.96 |
| ATOM | 5668 | N | ASP | B | 334 | 50.245 | 22.141 | 81.472 | 1.00 | 54.05 |
| ATOM | 5669 | CA | ASP | B | 334 | 49.850 | 22.306 | 82.865 | 1.00 | 58.15 |
| ATOM | 5670 | CB | ASP | B | 334 | 48.320 | 22.216 | 82.959 | 1.00 | 60.38 |
| ATOM | 5671 | CG | ASP | B | 334 | 47.751 | 20.972 | 82.262 | 1.00 | 63.85 |
| ATOM | 5672 | GD1 | ASP | B | 334 | 48.017 | 19.833 | 82.710 | 1.00 | 59.16 |
| ATOM | 5673 | OD2 | ASP | B | 334 | 47.033 | 21.138 | 81.252 | 1.00 | 59.71 |
| ATOM | 5674 | C | ASP | B | 334 | 50.506 | 21.207 | 83.701 | 1.00 | 55.47 |
| ATOM | 5675 | O | ASP | B | 334 | 49.833 | 20.291 | 84.171 | 1.00 | 54.08 |
| ATOM | 5676 | N | PHE | B | 335 | 51.816 | 21.307 | 83.906 | 1.00 | 54.60 |
| ATOM | 5677 | CA | PHE | B | 335 | 52.524 | 20.266 | 84.641 | 1.00 | 56.60 |
| ATOM | 5678 | CB | PHE | B | 335 | 53.718 | 19.784 | 83.811 | 1.00 | 53.01 |
| ATOM | 5679 | CG | PHE | B | 335 | 54.522 | 18.717 | 84.482 | 1.00 | 49.30 |
| ATOM | 5680 | CD1 | PHE | B | 335 | 53.898 | 17.589 | 85.008 | 1.00 | 45.61 |
| ATOM | 5681 | CD2 | PHE | B | 335 | 55.901 | 18.843 | 84.605 | 1.00 | 46.83 |
| ATOM | 5682 | CE1 | PHE | B | 335 | 54.637 | 16.600 | 85.651 | 1.00 | 45.95 |
| ATOM | 5683 | CE2 | PHE | B | 335 | 56.651 | 17.860 | 85.247 | 1.00 | 46.02 |
| ATOM | 5684 | CZ | PHE | B | 335 | 56.018 | 16.737 | 85.772 | 1.00 | 46.08 |
| ATOM | 5685 | C | PHE | B | 335 | 52.971 | 20.559 | 86.072 | 1.00 | 57.29 |
| ATOM | 5686 | O | PHE | B | 335 | 52.197 | 20.378 | 87.012 | 1.00 | 63.54 |
| ATOM | 5687 | N | GLU | B | 336 | 54.223 | 20.983 | 86.229 | 1.00 | 55.21 |
| ATOM | 5688 | CA | GLU | B | 336 | 54.818 | 21.286 | 87.535 | 1.00 | 60.30 |
| ATOM | 5689 | CB | GLU | B | 336 | 53.783 | 21.846 | 88.517 | 1.00 | 64.95 |
| ATOM | 5690 | CG | GLU | B | 336 | 54.375 | 22.225 | 89.867 | 1.00 | 71.50 |
| ATOM | 5691 | CD | GLU | B | 336 | 53.363 | 22.882 | 90.787 | 1.00 | 75.37 |
| ATOM | 5692 | OE1 | GLU | B | 336 | 52.796 | 23.925 | 90.394 | 1.00 | 75.32 |
| ATOM | 5693 | OE2 | GLU | B | 336 | 53.137 | 22.361 | 91.901 | 1.00 | 76.84 |
| ATOM | 5694 | C | GLU | B | 336 | 55.485 | 20.058 | 88.146 | 1.00 | 55.66 |
| ATOM | 5695 | O | GLU | B | 336 | 54.823 | 19.093 | 88.529 | 1.00 | 49.97 |
| ATOM | 5696 | N | GLU | B | 337 | 56.807 | 20.125 | 88.240 | 1.00 | 54.26 |
| ATOM | 5697 | CA | GLU | B | 337 | 57.630 | 19.047 | 88.767 | 1.00 | 54.35 |
| ATOM | 5698 | CB | GLU | B | 337 | 59.101 | 19.457 | 88.635 | 1.00 | 54.08 |
| ATOM | 5699 | CG | GLU | B | 337 | 60.074 | 18.315 | 88.514 | 1.00 | 54.15 |

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Figure 18-87

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5700 | CD | GLU | B | 337 | 59.856 | 17.496 | 87.259 | 1.00 | 48.94 |
| ATOM | 5701 | OE1 | GLU | B | 337 | 59.958 | 18.049 | 86.142 | 1.00 | 41.06 |
| ATOM | 5702 | OE2 | GLU | B | 337 | 59.581 | 16.292 | 87.391 | 1.00 | 50.23 |
| ATOM | 5703 | C | GLU | B | 337 | 57.278 | 18.740 | 90.227 | 1.00 | 55.08 |
| ATOM | 5704 | O | GLU | B | 337 | 57.130 | 19.651 | 91.039 | 1.00 | 54.51 |
| ATOM | 5705 | N | PHE | B | 338 | 57.140 | 17.458 | 90.557 | 1.00 | 56.20 |
| ATOM | 5706 | CA | PHE | B | 338 | 56.798 | 17.048 | 91.918 | 1.00 | 57.73 |
| ATOM | 5707 | CB | PHE | B | 338 | 56.713 | 15.527 | 92.020 | 1.00 | 58.47 |
| ATOM | 5708 | CG | PHE | B | 338 | 56.231 | 15.034 | 93.359 | 1.00 | 63.17 |
| ATOM | 5709 | CD1 | PHE | B | 338 | 54.882 | 15.096 | 93.696 | 1.00 | 64.86 |
| ATOM | 5710 | CD2 | PHE | B | 338 | 57.129 | 14.526 | 94.293 | 1.00 | 63.51 |
| ATOM | 5711 | CE1 | PHE | B | 338 | 54.434 | 14.656 | 94.943 | 1.00 | 65.25 |
| ATOM | 5712 | CE2 | PHE | B | 338 | 56.693 | 14.087 | 95.539 | 1.00 | 63.64 |
| ATOM | 5713 | CZ | PHE | B | 338 | 55.342 | 14.152 | 95.864 | 1.00 | 66.30 |
| ATOM | 5714 | C | PHE | B | 338 | 57.836 | 17.539 | 92.918 | 1.00 | 61.85 |
| ATOM | 5715 | O | PHE | B | 338 | 57.520 | 17.807 | 94.078 | 1.00 | 58.15 |
| ATOM | 5716 | N | ASP | B | 339 | 59.081 | 17.636 | 92.466 | 1.00 | 64.63 |
| ATOM | 5717 | CA | ASP | B | 339 | 60.167 | 18.099 | 93.316 | 1.00 | 67.53 |
| ATOM | 5718 | CB | ASP | B | 339 | 61.286 | 17.059 | 93.362 | 1.00 | 67.32 |
| ATOM | 5719 | CG | ASP | B | 339 | 62.474 | 17.524 | 94.174 | 1.00 | 68.13 |
| ATOM | 5720 | OD1 | ASP | B | 339 | 62.280 | 17.909 | 95.346 | 1.00 | 68.68 |
| ATOM | 5721 | OD2 | ASP | B | 339 | 63.603 | 17.502 | 93.646 | 1.00 | 69.03 |
| ATOM | 5722 | C | ASP | B | 339 | 60.718 | 19.435 | 92.829 | 1.00 | 69.03 |
| ATOM | 5723 | O | ASP | B | 339 | 61.211 | 19.545 | 91.708 | 1.00 | 67.54 |
| ATOM | 5724 | N | ASP | B | 340 | 60.626 | 20.442 | 93.693 | 1.00 | 72.19 |
| ATOM | 5725 | CA | ASP | B | 340 | 61.088 | 21.797 | 93.402 | 1.00 | 75.20 |
| ATOM | 5726 | CB | ASP | B | 340 | 61.113 | 22.623 | 94.689 | 1.00 | 77.04 |
| ATOM | 5727 | CG | ASP | B | 340 | 59.766 | 22.671 | 95.375 | 1.00 | 78.70 |
| ATOM | 5728 | OD1 | ASP | B | 340 | 58.803 | 23.181 | 94.763 | 1.00 | 79.66 |
| ATOM | 5729 | OD2 | ASP | B | 340 | 59.668 | 22.194 | 96.525 | 1.00 | 80.53 |
| ATOM | 5730 | C | ASP | B | 340 | 62.464 | 21.856 | 92.751 | 1.00 | 74.82 |
| ATOM | 5731 | O | ASP | B | 340 | 62.615 | 22.400 | 91.659 | 1.00 | 78.48 |
| ATOM | 5732 | N | GLU | B | 341 | 63.465 | 21.303 | 93.426 | 1.00 | 74.11 |
| ATOM | 5733 | CA | GLU | B | 341 | 64.827 | 21.312 | 92.907 | 1.00 | 76.25 |
| ATOM | 5734 | CB | GLU | B | 341 | 65.818 | 21.596 | 94.040 | 1.00 | 79.54 |
| ATOM | 5735 | CG | GLU | B | 341 | 67.277 | 21.653 | 93.596 | 1.00 | 82.33 |
| ATOM | 5736 | CD | GLU | B | 341 | 67.539 | 22.750 | 92.577 | 1.00 | 83.24 |
| ATOM | 5737 | OE1 | GLU | B | 341 | 67.333 | 23.937 | 92.910 | 1.00 | 85.25 |
| ATOM | 5738 | OE2 | GLU | B | 341 | 67.950 | 22.427 | 91.443 | 1.00 | 83.72 |
| ATOM | 5739 | C | GLU | B | 341 | 65.196 | 19.998 | 92.227 | 1.00 | 73.97 |
| ATOM | 5740 | O | GLU | B | 341 | 65.627 | 19.051 | 92.883 | 1.00 | 77.10 |
| ATOM | 5741 | N | VAL | B | 342 | 65.033 | 19.946 | 90.910 | 1.00 | 71.92 |
| ATOM | 5742 | CA | VAL | B | 342 | 65.354 | 18.744 | 90.151 | 1.00 | 68.51 |
| ATOM | 5743 | CB | VAL | B | 342 | 64.081 | 18.027 | 89.663 | 1.00 | 68.83 |
| ATOM | 5744 | CG1 | VAL | B | 342 | 63.268 | 17.552 | 90.837 | 1.00 | 67.57 |
| ATOM | 5745 | CG2 | VAL | B | 342 | 63.255 | 18.969 | 88.806 | 1.00 | 67.72 |
| ATOM | 5746 | C | VAL | B | 342 | 66.201 | 19.059 | 88.927 | 1.00 | 65.35 |
| ATOM | 5747 | O | VAL | B | 342 | 67.177 | 18.366 | 88.640 | 1.00 | 68.71 |
| ATOM | 5748 | N | ASP | B | 343 | 65.819 | 20.112 | 88.213 | 1.00 | 60.89 |
| ATOM | 5749 | CA | ASP | B | 343 | 66.514 | 20.520 | 86.998 | 1.00 | 58.89 |
| ATOM | 5750 | CB | ASP | B | 343 | 68.024 | 20.636 | 87.223 | 1.00 | 63.48 |
| ATOM | 5751 | CG | ASP | B | 343 | 68.763 | 21.070 | 85.966 | 1.00 | 66.69 |
| ATOM | 5752 | OD1 | ASP | B | 343 | 70.012 | 21.070 | 85.970 | 1.00 | 67.64 |
| ATOM | 5753 | OD2 | ASP | B | 343 | 68.089 | 21.420 | 84.973 | 1.00 | 65.42 |
| ATOM | 5754 | C | ASP | B | 343 | 66.264 | 19.499 | 85.900 | 1.00 | 53.17 |
| ATOM | 5755 | O | ASP | B | 343 | 66.993 | 18.516 | 85.766 | 1.00 | 49.70 |
| ATOM | 5756 | N | ARG | B | 344 | 65.216 | 19.735 | 85.124 | 1.00 | 50.24 |
| ATOM | 5757 | CA | ARG | B | 344 | 64.868 | 18.853 | 84.022 | 1.00 | 46.49 |
| ATOM | 5758 | CB | ARG | B | 344 | 63.467 | 18.269 | 84.228 | 1.00 | 42.41 |
| ATOM | 5759 | CG | ARG | B | 344 | 63.317 | 17.367 | 85.452 | 1.00 | 38.59 |
| ATOM | 5760 | CD | ARG | B | 344 | 64.344 | 16.246 | 85.432 | 1.00 | 37.12 |
| ATOM | 5761 | NE | ARG | B | 344 | 64.169 | 15.310 | 86.537 | 1.00 | 36.55 |
| ATOM | 5762 | CZ | ARG | B | 344 | 65.078 | 14.413 | 86.905 | 1.00 | 37.20 |
| ATOM | 5763 | NH1 | ARG | B | 344 | 66.234 | 14.331 | 86.259 | 1.00 | 33.53 |
| ATOM | 5764 | NH2 | ARG | B | 344 | 64.830 | 13.595 | 87.915 | 1.00 | 28.79 |
| ATOM | 5765 | C | ARG | B | 344 | 64.910 | 19.660 | 82.732 | 1.00 | 44.45 |

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Figure 18-88

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5766 | O | ARG | B | 344 | 64.328 | 19.269 | 81.720 | 1.00 | 38.73 |
| ATOM | 5767 | N | SER | B | 345 | 65.618 | 20.784 | 82.783 | 1.00 | 42.44 |
| ATOM | 5768 | CA | SER | B | 345 | 65.740 | 21.677 | 81.637 | 1.00 | 41.74 |
| ATOM | 5769 | CB | SER | B | 345 | 66.661 | 22.849 | 81.993 | 1.00 | 43.47 |
| ATOM | 5770 | OG | SER | B | 345 | 67.956 | 22.388 | 82.351 | 1.00 | 46.96 |
| ATOM | 5771 | C | SER | B | 345 | 66.244 | 20.981 | 80.375 | 1.00 | 36.32 |
| ATOM | 5772 | O | SER | B | 345 | 65.840 | 21.333 | 79.273 | 1.00 | 35.70 |
| ATOM | 5773 | N | TYR | B | 346 | 67.117 | 19.992 | 80.534 | 1.00 | 33.93 |
| ATOM | 5774 | CA | TYR | B | 346 | 67.661 | 19.264 | 79.391 | 1.00 | 34.77 |
| ATOM | 5775 | CB | TYR | B | 346 | 68.660 | 18.206 | 79.877 | 1.00 | 36.09 |
| ATOM | 5776 | CG | TYR | B | 346 | 68.054 | 17.146 | 80.774 | 1.00 | 34.27 |
| ATOM | 5777 | CD1 | TYR | B | 346 | 67.433 | 16.013 | 80.240 | 1.00 | 37.62 |
| ATOM | 5778 | CE1 | TYR | B | 346 | 66.843 | 15.048 | 81.077 | 1.00 | 36.73 |
| ATOM | 5779 | CD2 | TYR | B | 346 | 68.072 | 17.294 | 82.157 | 1.00 | 36.40 |
| ATOM | 5780 | CE2 | TYR | B | 346 | 67.489 | 16.344 | 82.999 | 1.00 | 36.54 |
| ATOM | 5781 | CZ | TYR | B | 346 | 66.878 | 15.228 | 82.457 | 1.00 | 36.54 |
| ATOM | 5782 | OH | TYR | B | 346 | 66.310 | 14.306 | 83.306 | 1.00 | 33.35 |
| ATOM | 5783 | C | TYR | B | 346 | 66.563 | 18.599 | 78.570 | 1.00 | 36.26 |
| ATOM | 5784 | O | TYR | B | 346 | 66.719 | 18.385 | 77.367 | 1.00 | 40.50 |
| ATOM | 5785 | N | MET | B | 347 | 65.445 | 18.282 | 79.214 | 1.00 | 32.72 |
| ATOM | 5786 | CA | MET | B | 347 | 64.346 | 17.628 | 78.516 | 1.00 | 35.43 |
| ATOM | 5787 | CB | MET | B | 347 | 63.280 | 17.164 | 79.513 | 1.00 | 34.36 |
| ATOM | 5788 | CG | MET | B | 347 | 63.819 | 16.292 | 80.635 | 1.00 | 28.32 |
| ATOM | 5789 | SD | MET | B | 347 | 62.515 | 15.604 | 81.669 | 1.00 | 34.47 |
| ATOM | 5790 | CE | MET | B | 347 | 61.654 | 17.027 | 82.142 | 1.00 | 39.60 |
| ATOM | 5791 | C | MET | B | 347 | 63.701 | 18.525 | 77.465 | 1.00 | 39.04 |
| ATOM | 5792 | O | MET | B | 347 | 63.060 | 18.029 | 76.540 | 1.00 | 37.38 |
| ATOM | 5793 | N | LEU | B | 348 | 63.857 | 19.839 | 77.606 | 1.00 | 39.21 |
| ATOM | 5794 | CA | LEU | B | 348 | 63.272 | 20.773 | 76.645 | 1.00 | 40.81 |
| ATOM | 5795 | CB | LEU | B | 348 | 62.806 | 22.058 | 77.339 | 1.00 | 36.87 |
| ATOM | 5796 | CG | LEU | B | 348 | 61.690 | 21.975 | 78.384 | 1.00 | 42.66 |
| ATOM | 5797 | CD1 | LEU | B | 348 | 61.507 | 23.337 | 79.032 | 1.00 | 43.41 |
| ATOM | 5798 | CD2 | LEU | B | 348 | 60.391 | 21.511 | 77.741 | 1.00 | 40.47 |
| ATOM | 5799 | C | LEU | B | 348 | 64.289 | 21.133 | 75.573 | 1.00 | 41.13 |
| ATOM | 5800 | O | LEU | B | 348 | 64.018 | 21.968 | 74.711 | 1.00 | 38.93 |
| ATOM | 5801 | N | GLU | B | 349 | 65.455 | 20.495 | 75.632 | 1.00 | 37.70 |
| ATOM | 5802 | CA | GLU | B | 349 | 66.527 | 20.757 | 74.681 | 1.00 | 42.48 |
| ATOM | 5803 | CB | GLU | B | 349 | 67.856 | 20.953 | 75.422 | 1.00 | 45.02 |
| ATOM | 5804 | CG | GLU | B | 349 | 67.834 | 22.035 | 76.493 | 1.00 | 53.82 |
| ATOM | 5805 | CD | GLU | B | 349 | 67.483 | 23.402 | 75.938 | 1.00 | 57.46 |
| ATOM | 5806 | OE1 | GLU | B | 349 | 68.211 | 23.885 | 75.044 | 1.00 | 59.62 |
| ATOM | 5807 | OE2 | GLU | B | 349 | 66.480 | 23.993 | 76.397 | 1.00 | 57.91 |
| ATOM | 5808 | C | GLU | B | 349 | 66.709 | 19.638 | 73.664 | 1.00 | 43.57 |
| ATOM | 5809 | O | GLU | B | 349 | 66.577 | 19.849 | 72.459 | 1.00 | 41.26 |
| ATOM | 5810 | N | THR | B | 350 | 67.027 | 18.448 | 74.161 | 1.00 | 41.95 |
| ATOM | 5811 | CA | THR | B | 350 | 67.264 | 17.299 | 73.298 | 1.00 | 40.02 |
| ATOM | 5812 | CB | THR | B | 350 | 68.689 | 16.775 | 73.504 | 1.00 | 43.08 |
| ATOM | 5813 | OG1 | THR | B | 350 | 68.894 | 16.490 | 74.894 | 1.00 | 41.07 |
| ATOM | 5814 | CG2 | THR | B | 350 | 69.703 | 17.816 | 73.049 | 1.00 | 45.05 |
| ATOM | 5815 | C | THR | B | 350 | 66.278 | 16.154 | 73.510 | 1.00 | 37.56 |
| ATOM | 5816 | O | THR | B | 350 | 65.754 | 15.966 | 74.611 | 1.00 | 33.64 |
| ATOM | 5817 | N | LEU | B | 351 | 66.043 | 15.391 | 72.445 | 1.00 | 32.86 |
| ATOM | 5818 | CA | LEU | B | 351 | 65.126 | 14.260 | 72.475 | 1.00 | 35.00 |
| ATOM | 5819 | CB | LEU | B | 351 | 64.776 | 13.810 | 71.053 | 1.00 | 31.61 |
| ATOM | 5820 | CG | LEU | B | 351 | 63.709 | 14.601 | 70.312 | 1.00 | 35.31 |
| ATOM | 5821 | CD1 | LEU | B | 351 | 63.552 | 14.064 | 68.904 | 1.00 | 37.88 |
| ATOM | 5822 | CD2 | LEU | B | 351 | 62.397 | 14.474 | 71.068 | 1.00 | 39.36 |
| ATOM | 5823 | C | LEU | B | 351 | 65.662 | 13.065 | 73.240 | 1.00 | 33.33 |
| ATOM | 5824 | O | LEU | B | 351 | 64.956 | 12.469 | 74.046 | 1.00 | 31.48 |
| ATOM | 5825 | N | LYS | B | 352 | 66.915 | 12.720 | 72.981 | 1.00 | 29.58 |
| ATOM | 5826 | CA | LYS | B | 352 | 67.527 | 11.576 | 73.633 | 1.00 | 36.77 |
| ATOM | 5827 | CB | LYS | B | 352 | 68.457 | 10.864 | 72.647 | 1.00 | 34.32 |
| ATOM | 5828 | CG | LYS | B | 352 | 67.777 | 10.563 | 71.326 | 1.00 | 39.29 |
| ATOM | 5829 | CD | LYS | B | 352 | 68.703 | 9.949 | 70.294 | 1.00 | 42.25 |
| ATOM | 5830 | CE | LYS | B | 352 | 69.110 | 8.541 | 70.655 | 1.00 | 46.22 |
| ATOM | 5831 | NZ | LYS | B | 352 | 69.831 | 7.905 | 69.516 | 1.00 | 44.15 |

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Figure 18-89

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5832 | C | LYS | B | 352 | 68.295 | 11.983 | 74.878 | 1.00 | 36.30 |
| ATOM | 5833 | O | LYS | B | 352 | 69.086 | 12.931 | 74.865 | 1.00 | 36.65 |
| ATOM | 5834 | N | ASP | B | 353 | 68.049 | 11.275 | 75.967 | 1.00 | 30.01 |
| ATOM | 5835 | CA | ASP | B | 353 | 68.757 | 11.569 | 77.188 | 1.00 | 33.99 |
| ATOM | 5836 | CB | ASP | B | 353 | 67.852 | 11.308 | 78.394 | 1.00 | 38.57 |
| ATOM | 5837 | CG | ASP | B | 353 | 67.134 | 9.986 | 78.315 | 1.00 | 43.90 |
| ATOM | 5838 | OD1 | ASP | B | 353 | 66.034 | 9.851 | 78.926 | 1.00 | 22.39 |
| ATOM | 5839 | OD2 | ASP | B | 353 | 67.679 | 9.078 | 77.649 | 1.00 | 50.42 |
| ATOM | 5840 | C | ASP | B | 353 | 70.022 | 10.723 | 77.202 | 1.00 | 35.83 |
| ATOM | 5841 | O | ASP | B | 353 | 70.189 | 9.833 | 76.368 | 1.00 | 23.71 |
| ATOM | 5842 | N | PRO | B | 354 | 70.954 | 11.025 | 78.116 | 1.00 | 36.36 |
| ATOM | 5843 | CD | PRO | B | 354 | 70.928 | 12.093 | 79.132 | 1.00 | 38.28 |
| ATOM | 5844 | CA | PRO | B | 354 | 72.205 | 10.277 | 78.212 | 1.00 | 33.62 |
| ATOM | 5845 | CB | PRO | B | 354 | 73.003 | 11.104 | 79.213 | 1.00 | 34.46 |
| ATOM | 5846 | CG | PRO | B | 354 | 71.896 | 11.556 | 80.164 | 1.00 | 38.08 |
| ATOM | 5847 | C | PRO | B | 354 | 71.924 | 8.883 | 78.733 | 1.00 | 33.62 |
| ATOM | 5848 | O | PRO | B | 354 | 70.894 | 8.643 | 79.366 | 1.00 | 24.82 |
| ATOM | 5849 | N | TRP | B | 355 | 72.833 | 7.954 | 78.468 | 1.00 | 31.76 |
| ATOM | 5850 | CA | TRP | B | 355 | 72.635 | 6.611 | 78.969 | 1.00 | 30.01 |
| ATOM | 5851 | CB | TRP | B | 355 | 73.653 | 5.655 | 78.359 | 1.00 | 34.02 |
| ATOM | 5852 | CG | TRP | B | 355 | 73.025 | 4.378 | 77.910 | 1.00 | 44.37 |
| ATOM | 5853 | CD2 | TRP | B | 355 | 73.263 | 3.072 | 78.436 | 1.00 | 45.39 |
| ATOM | 5854 | CE2 | TRP | B | 355 | 72.418 | 2.177 | 77.734 | 1.00 | 44.31 |
| ATOM | 5855 | CE3 | TRP | B | 355 | 74.107 | 2.569 | 79.432 | 1.00 | 47.19 |
| ATOM | 5856 | CD1 | TRP | B | 355 | 72.073 | 4.230 | 76.935 | 1.00 | 42.18 |
| ATOM | 5857 | NE1 | TRP | B | 355 | 71.704 | 2.910 | 76.826 | 1.00 | 37.84 |
| ATOM | 5858 | CZ2 | TRP | B | 355 | 72.395 | 0.808 | 77.999 | 1.00 | 44.97 |
| ATOM | 5859 | CZ3 | TRP | B | 355 | 74.084 | 1.207 | 79.694 | 1.00 | 50.83 |
| ATOM | 5860 | CH2 | TRP | B | 355 | 73.231 | 0.341 | 78.979 | 1.00 | 48.73 |
| ATOM | 5861 | C | TRP | B | 355 | 72.819 | 6.685 | 80.485 | 1.00 | 30.87 |
| ATOM | 5862 | O | TRP | B | 355 | 73.622 | 7.474 | 80.981 | 1.00 | 26.93 |
| ATOM | 5863 | N | ARG | B | 356 | 72.061 | 5.880 | 81.218 | 1.00 | 24.96 |
| ATOM | 5864 | CA | ARG | B | 356 | 72.147 | 5.848 | 82.671 | 1.00 | 23.57 |
| ATOM | 5865 | CB | ARG | B | 356 | 70.811 | 6.319 | 83.257 | 1.00 | 24.71 |
| ATOM | 5866 | CG | ARG | B | 356 | 70.534 | 7.795 | 82.941 | 1.00 | 23.66 |
| ATOM | 5867 | CD | ARG | B | 356 | 69.067 | 8.212 | 83.055 | 1.00 | 20.14 |
| ATOM | 5868 | NE | ARG | B | 356 | 68.926 | 9.610 | 82.642 | 1.00 | 20.59 |
| ATOM | 5869 | CZ | ARG | B | 356 | 67.787 | 10.192 | 82.288 | 1.00 | 25.41 |
| ATOM | 5870 | NH1 | ARG | B | 356 | 66.644 | 9.508 | 82.287 | 1.00 | 17.01 |
| ATOM | 5871 | NH2 | ARG | B | 356 | 67.796 | 11.464 | 81.910 | 1.00 | 20.07 |
| ATOM | 5872 | C | ARG | B | 356 | 72.481 | 4.410 | 83.085 | 1.00 | 26.57 |
| ATOM | 5873 | O | ARG | B | 356 | 71.610 | 3.641 | 83.485 | 1.00 | 23.02 |
| ATOM | 5874 | N | GLY | B | 357 | 73.761 | 4.063 | 82.978 | 1.00 | 23.92 |
| ATOM | 5875 | CA | GLY | B | 357 | 74.186 | 2.712 | 83.294 | 1.00 | 25.54 |
| ATOM | 5876 | C | GLY | B | 357 | 74.796 | 2.464 | 84.657 | 1.00 | 24.35 |
| ATOM | 5877 | O | GLY | B | 357 | 74.523 | 3.161 | 85.628 | 1.00 | 25.88 |
| ATOM | 5878 | N | GLY | B | 358 | 75.638 | 1.444 | 84.718 | 1.00 | 24.32 |
| ATOM | 5879 | CA | GLY | B | 358 | 76.282 | 1.070 | 85.960 | 1.00 | 23.56 |
| ATOM | 5880 | C | GLY | B | 358 | 76.412 | -0.441 | 85.924 | 1.00 | 29.26 |
| ATOM | 5881 | O | GLY | B | 358 | 76.146 | -1.051 | 84.889 | 1.00 | 23.71 |
| ATOM | 5882 | N | GLU | B | 359 | 76.814 | -1.051 | 87.033 | 1.00 | 27.64 |
| ATOM | 5883 | CA | GLU | B | 359 | 76.955 | -2.503 | 87.078 | 1.00 | 32.16 |
| ATOM | 5884 | CB | GLU | B | 359 | 77.822 | -2.936 | 88.265 | 1.00 | 30.40 |
| ATOM | 5885 | CG | GLU | B | 359 | 77.125 | -2.772 | 89.601 | 1.00 | 31.23 |
| ATOM | 5886 | CD | GLU | B | 359 | 77.844 | -3.479 | 90.741 | 1.00 | 37.96 |
| ATOM | 5887 | OE1 | GLU | B | 359 | 77.287 | -3.521 | 91.861 | 1.00 | 33.89 |
| ATOM | 5888 | OE2 | GLU | B | 359 | 78.959 | -3.990 | 90.520 | 1.00 | 37.40 |
| ATOM | 5889 | C | GLU | B | 359 | 75.571 | -3.122 | 87.261 | 1.00 | 31.35 |
| ATOM | 5890 | O | GLU | B | 359 | 74.612 | -2.429 | 87.588 | 1.00 | 25.15 |
| ATOM | 5891 | N | VAL | B | 360 | 75.482 | -4.428 | 87.053 | 1.00 | 29.61 |
| ATOM | 5892 | CA | VAL | B | 360 | 74.230 | -5.147 | 87.251 | 1.00 | 26.21 |
| ATOM | 5893 | CB | VAL | B | 360 | 74.035 | -6.270 | 86.200 | 1.00 | 28.47 |
| ATOM | 5894 | CG1 | VAL | B | 360 | 72.764 | -7.045 | 86.492 | 1.00 | 22.74 |
| ATOM | 5895 | CG2 | VAL | B | 360 | 73.969 | -5.670 | 84.796 | 1.00 | 29.70 |
| ATOM | 5896 | C | VAL | B | 360 | 74.342 | -5.784 | 88.625 | 1.00 | 26.00 |
| ATOM | 5897 | O | VAL | B | 360 | 75.150 | -6.693 | 88.821 | 1.00 | 27.55 |

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Figure 18-90

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 5898 | N | ARG | B | 361 | 73.553 | -5.289 | 89.575 | 1.00 | 26.45 |
| ATOM | 5899 | CA | ARG | B | 361 | 73.558 | -5.821 | 90.935 | 1.00 | 28.47 |
| ATOM | 5900 | CB | ARG | B | 361 | 72.479 | -5.146 | 91.787 | 1.00 | 30.55 |
| ATOM | 5901 | CG | ARG | B | 361 | 72.937 | -3.877 | 92.485 | 1.00 | 32.61 |
| ATOM | 5902 | CD | ARG | B | 361 | 71.749 | -3.163 | 93.117 | 1.00 | 35.00 |
| ATOM | 5903 | NE | ARG | B | 361 | 70.858 | -2.617 | 92.094 | 1.00 | 30.31 |
| ATOM | 5904 | CZ | ARG | B | 361 | 69.753 | -1.925 | 92.350 | 1.00 | 29.45 |
| ATOM | 5905 | NH1 | ARG | B | 361 | 69.385 | -1.689 | 93.605 | 1.00 | 18.49 |
| ATOM | 5906 | NH2 | ARG | B | 361 | 69.041 | -1.428 | 91.348 | 1.00 | 30.49 |
| ATOM | 5907 | C | ARG | B | 361 | 73.351 | -7.322 | 91.001 | 1.00 | 30.17 |
| ATOM | 5908 | O | ARG | B | 361 | 72.665 | -7.910 | 90.168 | 1.00 | 23.60 |
| ATOM | 5909 | N | LYS | B | 362 | 73.949 | -7.922 | 92.022 | 1.00 | 33.09 |
| ATOM | 5910 | CA | LYS | B | 362 | 73.864 | -9.351 | 92.272 | 1.00 | 36.94 |
| ATOM | 5911 | CB | LYS | B | 362 | 74.687 | -9.706 | 93.513 | 1.00 | 40.24 |
| ATOM | 5912 | CG | LYS | B | 362 | 76.190 | -9.527 | 93.337 | 1.00 | 52.55 |
| ATOM | 5913 | CD | LYS | B | 362 | 76.571 | -8.126 | 92.849 | 1.00 | 56.65 |
| ATOM | 5914 | CE | LYS | B | 362 | 76.149 | -7.032 | 93.819 | 1.00 | 53.39 |
| ATOM | 5915 | NZ | LYS | B | 362 | 76.553 | -5.680 | 93.341 | 1.00 | 48.87 |
| ATOM | 5916 | C | LYS | B | 362 | 72.427 | -9.826 | 92.463 | 1.00 | 32.84 |
| ATOM | 5917 | O | LYS | B | 362 | 72.045 | -10.867 | 91.938 | 1.00 | 28.27 |
| ATOM | 5918 | N | GLU | B | 363 | 71.628 | -9.075 | 93.215 | 1.00 | 34.67 |
| ATOM | 5919 | CA | GLU | B | 363 | 70.245 | -9.493 | 93.435 | 1.00 | 35.72 |
| ATOM | 5920 | CB | GLU | B | 363 | 69.519 | -8.532 | 94.390 | 1.00 | 36.04 |
| ATOM | 5921 | CG | GLU | B | 363 | 69.502 | -7.077 | 93.977 | 1.00 | 44.81 |
| ATOM | 5922 | CD | GLU | B | 363 | 68.859 | -6.186 | 95.033 | 1.00 | 52.14 |
| ATOM | 5923 | OE1 | GLU | B | 363 | 67.661 | -6.370 | 95.341 | 1.00 | 48.46 |
| ATOM | 5924 | OE2 | GLU | B | 363 | 69.562 | -5.300 | 95.566 | 1.00 | 57.31 |
| ATOM | 5925 | C | GLU | B | 363 | 69.501 | -9.619 | 92.111 | 1.00 | 30.68 |
| ATOM | 5926 | O | GLU | B | 363 | 68.695 | -10.530 | 91.944 | 1.00 | 30.45 |
| ATOM | 5927 | N | VAL | B | 364 | 69.784 | -8.724 | 91.166 | 1.00 | 26.19 |
| ATOM | 5928 | CA | VAL | B | 364 | 69.138 | -8.789 | 89.852 | 1.00 | 24.65 |
| ATOM | 5929 | CB | VAL | B | 364 | 69.536 | -7.599 | 88.958 | 1.00 | 23.49 |
| ATOM | 5930 | CG1 | VAL | B | 364 | 68.924 | -7.770 | 87.563 | 1.00 | 21.01 |
| ATOM | 5931 | CG2 | VAL | B | 364 | 69.049 | -6.293 | 89.587 | 1.00 | 23.08 |
| ATOM | 5932 | C | VAL | B | 364 | 69.530 | -10.083 | 89.144 | 1.00 | 23.19 |
| ATOM | 5933 | O | VAL | B | 364 | 68.691 | -10.749 | 88.542 | 1.00 | 23.06 |
| ATOM | 5934 | N | LYS | B | 365 | 70.810 | -10.436 | 89.216 | 1.00 | 27.15 |
| ATOM | 5935 | CA | LYS | B | 365 | 71.296 | -11.668 | 88.594 | 1.00 | 29.18 |
| ATOM | 5936 | CB | LYS | B | 365 | 72.821 | -11.758 | 88.704 | 1.00 | 28.61 |
| ATOM | 5937 | CG | LYS | B | 365 | 73.554 | -10.617 | 88.030 | 1.00 | 30.27 |
| ATOM | 5938 | CD | LYS | B | 365 | 75.074 | -10.768 | 88.154 | 1.00 | 32.58 |
| ATOM | 5939 | CE | LYS | B | 365 | 75.790 | -9.587 | 87.516 | 1.00 | 29.13 |
| ATOM | 5940 | NZ | LYS | B | 365 | 77.271 | -9.689 | 87.606 | 1.00 | 35.17 |
| ATOM | 5941 | C | LYS | B | 365 | 70.666 | -12.879 | 89.276 | 1.00 | 25.30 |
| ATOM | 5942 | O | LYS | B | 365 | 70.282 | -13.837 | 88.613 | 1.00 | 26.81 |
| ATOM | 5943 | N | ASP | B | 366 | 70.559 | -12.831 | 90.604 | 1.00 | 26.10 |
| ATOM | 5944 | CA | ASP | B | 366 | 69.963 | -13.938 | 91.347 | 1.00 | 28.29 |
| ATOM | 5945 | CB | ASP | B | 366 | 70.105 | -13.731 | 92.859 | 1.00 | 29.44 |
| ATOM | 5946 | CG | ASP | B | 366 | 71.557 | -13.669 | 93.311 | 1.00 | 32.95 |
| ATOM | 5947 | OD1 | ASP | B | 366 | 72.446 | -14.099 | 92.551 | 1.00 | 26.37 |
| ATOM | 5948 | OD2 | ASP | B | 366 | 71.811 | -13.216 | 94.442 | 1.00 | 35.26 |
| ATOM | 5949 | C | ASP | B | 366 | 68.487 | -14.110 | 90.986 | 1.00 | 28.61 |
| ATOM | 5950 | O | ASP | B | 366 | 68.000 | -15.231 | 90.869 | 1.00 | 27.00 |
| ATOM | 5951 | N | THR | B | 367 | 67.777 | -13.002 | 90.801 | 1.00 | 28.63 |
| ATOM | 5952 | CA | THR | B | 367 | 66.365 | -13.080 | 90.438 | 1.00 | 27.35 |
| ATOM | 5953 | CB | THR | B | 367 | 65.726 | -11.683 | 90.359 | 1.00 | 27.63 |
| ATOM | 5954 | OG1 | THR | B | 367 | 65.771 | -11.068 | 91.656 | 1.00 | 28.12 |
| ATOM | 5955 | CG2 | THR | B | 367 | 64.280 | -11.786 | 89.890 | 1.00 | 22.94 |
| ATOM | 5956 | C | THR | B | 367 | 66.197 | -13.782 | 89.094 | 1.00 | 25.46 |
| ATOM | 5957 | O | THR | B | 367 | 65.389 | -14.693 | 88.964 | 1.00 | 24.48 |
| ATOM | 5958 | N | LEU | B | 368 | 66.962 | -13.361 | 88.092 | 1.00 | 23.33 |
| ATOM | 5959 | CA | LEU | B | 368 | 66.857 | -13.990 | 86.785 | 1.00 | 28.99 |
| ATOM | 5960 | CB | LEU | B | 368 | 67.719 | -13.256 | 85.759 | 1.00 | 27.67 |
| ATOM | 5961 | CG | LEU | B | 368 | 67.060 | -12.070 | 85.046 | 1.00 | 29.47 |
| ATOM | 5962 | CD1 | LEU | B | 368 | 65.923 | -12.607 | 84.195 | 1.00 | 32.45 |
| ATOM | 5963 | CD2 | LEU | B | 368 | 66.546 | -11.027 | 86.043 | 1.00 | 19.43 |

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Figure 18-91

| | | | | | | | | |
|--------|------|-----|-----------|--------|---------|---------|------|-------|
| ATOM | 5964 | C | LEU B 368 | 67.262 | -15.454 | 86.888 | 1.00 | 32.40 |
| ATOM | 5965 | O | LEU B 368 | 66.726 | -16.309 | 86.179 | 1.00 | 31.80 |
| ATOM | 5966 | N | GLU B 369 | 68.212 | -15.735 | 87.774 | 1.00 | 33.59 |
| ATOM | 5967 | CA | GLU B 369 | 68.656 | -17.101 | 88.003 | 1.00 | 39.68 |
| ATOM | 5968 | CB | GLU B 369 | 69.736 | -17.141 | 89.082 | 1.00 | 42.61 |
| ATOM | 5969 | CG | GLU B 369 | 71.133 | -17.138 | 88.537 | 1.00 | 50.65 |
| ATOM | 5970 | CD | GLU B 369 | 71.469 | -18.443 | 87.842 | 1.00 | 55.81 |
| ATOM | 5971 | OE1 | GLU B 369 | 72.589 | -18.561 | 87.299 | 1.00 | 57.42 |
| ATOM | 5972 | OE2 | GLU B 369 | 70.610 | -19.353 | 87.841 | 1.00 | 58.37 |
| ATOM | 5973 | C | GLU B 369 | 67.479 | -17.954 | 88.442 | 1.00 | 34.94 |
| ATOM | 5974 | O | GLU B 369 | 67.190 | -18.974 | 87.827 | 1.00 | 32.71 |
| ATOM | 5975 | N | LYS B 370 | 66.805 | -17.541 | 89.512 | 1.00 | 34.92 |
| ATOM | 5976 | CA | LYS B 370 | 65.656 | -18.295 | 89.993 | 1.00 | 35.12 |
| ATOM | 5977 | CB | LYS B 370 | 65.061 | -17.679 | 91.268 | 1.00 | 37.39 |
| ATOM | 5978 | CG | LYS B 370 | 65.879 | -17.916 | 92.532 | 1.00 | 44.70 |
| ATOM | 5979 | CD | LYS B 370 | 66.781 | -16.741 | 92.892 | 1.00 | 48.10 |
| ATOM | 5980 | CE | LYS B 370 | 65.956 | -15.537 | 93.346 | 1.00 | 47.82 |
| ATOM | 5981 | NZ | LYS B 370 | 66.804 | -14.387 | 93.786 | 1.00 | 45.41 |
| ATOM | 5982 | C | LYS B 370 | 64.581 | -18.375 | 88.930 | 1.00 | 33.21 |
| ATOM | 5983 | O | LYS B 370 | 63.937 | -19.409 | 88.773 | 1.00 | 29.52 |
| ATOM | 5984 | N | ALA B 371 | 64.390 | -17.288 | 88.191 | 1.00 | 31.62 |
| ATOM | 5985 | CA | ALA B 371 | 63.368 | -17.274 | 87.153 | 1.00 | 37.19 |
| ATOM | 5986 | CB | ALA B 371 | 63.392 | -15.938 | 86.403 | 1.00 | 35.65 |
| ATOM | 5987 | C | ALA B 371 | 63.572 | -18.431 | 86.181 | 1.00 | 37.79 |
| ATOM | 5988 | O | ALA B 371 | 62.627 | -19.137 | 85.838 | 1.00 | 34.46 |
| ATOM | 5989 | N | LYS B 372 | 64.810 | -18.644 | 85.759 | 1.00 | 40.10 |
| ATOM | 5990 | CA | LYS B 372 | 65.147 | -19.698 | 84.792 | 1.00 | 40.46 |
| ATOM | 5991 | C | LYS B 372 | 64.746 | -21.066 | 85.348 | 1.00 | 43.15 |
| ATOM | 5992 | O | LYS B 372 | 64.757 | -22.053 | 84.591 | 1.00 | 43.57 |
| ATOM | 5993 | CB | LYS B 372 | 66.654 | -19.694 | 84.517 | 1.00 | 40.51 |
| ATOM | 5994 | CG | LYS B 372 | 67.029 | -18.925 | 83.248 | 1.00 | 20.00 |
| ATOM | 5995 | CD | LYS B 372 | 68.352 | -19.390 | 82.635 | 1.00 | 20.00 |
| ATOM | 5996 | CE | LYS B 372 | 68.544 | -20.907 | 82.706 | 1.00 | 20.00 |
| ATOM | 5997 | NZ | LYS B 372 | 69.814 | -21.354 | 82.116 | 1.00 | 20.00 |
| ATOM | 5998 | N | ALA B 373 | 64.412 | -21.159 | 86.624 | 1.00 | 47.80 |
| ATOM | 5999 | CA | ALA B 373 | 64.014 | -22.425 | 87.239 | 1.00 | 49.71 |
| ATOM | 6000 | CB | ALA B 373 | 64.762 | -22.639 | 88.546 | 1.00 | 48.25 |
| ATOM | 6001 | C | ALA B 373 | 62.515 | -22.443 | 87.494 | 1.00 | 53.38 |
| ATOM | 6002 | O | ALA B 373 | 61.844 | -23.313 | 86.903 | 1.00 | 58.01 |
| ATOM | 6003 | OXT | ALA B 373 | 62.029 | -21.589 | 88.269 | 1.00 | 55.13 |
| HETATM | 2991 | ZN | ZN C 1 | 49.660 | 9.211 | 109.302 | 1.00 | 32.54 |
| HETATM | 2992 | O1 | TSA D 2 | 47.669 | 8.189 | 109.464 | 1.00 | 28.76 |
| HETATM | 2993 | O2 | TSA D 2 | 49.952 | 6.981 | 108.340 | 1.00 | 25.81 |
| HETATM | 2994 | O3 | TSA D 2 | 52.458 | 5.101 | 101.667 | 1.00 | 36.93 |
| HETATM | 2995 | N1 | TSA D 2 | 47.800 | 7.789 | 108.131 | 1.00 | 31.21 |
| HETATM | 2996 | N2 | TSA D 2 | 53.013 | -1.329 | 101.259 | 1.00 | 30.57 |
| HETATM | 2997 | C1 | TSA D 2 | 51.859 | 2.799 | 101.610 | 1.00 | 28.47 |
| HETATM | 2998 | C2 | TSA D 2 | 50.907 | 1.769 | 101.666 | 1.00 | 25.57 |
| HETATM | 2999 | C3 | TSA D 2 | 51.241 | 0.419 | 101.551 | 1.00 | 21.68 |
| HETATM | 3000 | C4 | TSA D 2 | 52.626 | 0.026 | 101.366 | 1.00 | 23.11 |
| HETATM | 3001 | C5 | TSA D 2 | 53.589 | 1.080 | 101.303 | 1.00 | 25.02 |
| HETATM | 3002 | C6 | TSA D 2 | 53.218 | 2.408 | 101.418 | 1.00 | 29.24 |
| HETATM | 3003 | C7 | TSA D 2 | 51.572 | 4.261 | 101.734 | 1.00 | 32.98 |
| HETATM | 3004 | C8 | TSA D 2 | 50.108 | 4.726 | 101.996 | 1.00 | 29.05 |
| HETATM | 3005 | C9 | TSA D 2 | 50.052 | 5.421 | 103.338 | 1.00 | 28.13 |
| HETATM | 3006 | C10 | TSA D 2 | 49.060 | 5.357 | 104.279 | 1.00 | 25.99 |
| HETATM | 3007 | C11 | TSA D 2 | 49.315 | 6.155 | 105.504 | 1.00 | 32.05 |
| HETATM | 3008 | C12 | TSA D 2 | 48.515 | 6.184 | 106.595 | 1.00 | 27.37 |
| HETATM | 3009 | C13 | TSA D 2 | 48.855 | 6.994 | 107.756 | 1.00 | 29.02 |
| HETATM | 3010 | C14 | TSA D 2 | 49.680 | 5.693 | 100.864 | 1.00 | 30.21 |
| HETATM | 3011 | C15 | TSA D 2 | 47.776 | 4.545 | 104.132 | 1.00 | 30.60 |
| HETATM | 3012 | C17 | TSA D 2 | 54.438 | -1.703 | 101.139 | 1.00 | 23.45 |
| HETATM | 3013 | C16 | TSA D 2 | 52.044 | -2.416 | 101.316 | 1.00 | 23.15 |
| HETATM | 6004 | ZN | ZN E 1 | 52.949 | 1.842 | 85.681 | 1.00 | 28.19 |
| HETATM | 6005 | O1 | TSA F 2 | 50.964 | 0.911 | 85.428 | 1.00 | 24.72 |
| HETATM | 6006 | O2 | TSA F 2 | 51.255 | 3.324 | 86.654 | 1.00 | 30.24 |

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Figure 18-92

| | | | | | | | | | |
|-------------|-----|-----|---|----|--------|---------|---------|------|-------|
| HETATM 6007 | O3 | TSA | F | 2 | 51.569 | 6.512 | 93.219 | 1.00 | 27.89 |
| HETATM 6008 | N1 | TSA | F | 2 | 50.347 | 1.221 | 86.634 | 1.00 | 27.23 |
| HETATM 6009 | N2 | TSA | F | 2 | 47.061 | 11.139 | 93.713 | 1.00 | 16.24 |
| HETATM 6010 | C1 | TSA | F | 2 | 49.443 | 7.579 | 93.304 | 1.00 | 27.18 |
| HETATM 6011 | C2 | TSA | F | 2 | 48.035 | 7.529 | 93.267 | 1.00 | 25.98 |
| HETATM 6012 | C3 | TSA | F | 2 | 47.227 | 8.657 | 93.398 | 1.00 | 24.59 |
| HETATM 6013 | C4 | TSA | F | 2 | 47.837 | 9.971 | 93.583 | 1.00 | 25.75 |
| HETATM 6014 | C5 | TSA | F | 2 | 49.274 | 10.017 | 93.626 | 1.00 | 26.53 |
| HETATM 6015 | C6 | TSA | F | 2 | 50.041 | 8.869 | 93.495 | 1.00 | 28.36 |
| HETATM 6016 | C7 | TSA | F | 2 | 50.349 | 6.405 | 93.167 | 1.00 | 25.27 |
| HETATM 6017 | C8 | TSA | F | 2 | 49.716 | 5.006 | 92.905 | 1.00 | 24.18 |
| HETATM 6018 | C9 | TSA | F | 2 | 50.134 | 4.552 | 91.518 | 1.00 | 27.20 |
| HETATM 6019 | C10 | TSA | F | 2 | 49.419 | 3.807 | 90.616 | 1.00 | 30.21 |
| HETATM 6020 | C11 | TSA | F | 2 | 50.118 | 3.553 | 89.327 | 1.00 | 27.18 |
| HETATM 6021 | C12 | TSA | F | 2 | 49.762 | 2.624 | 88.409 | 1.00 | 23.47 |
| HETATM 6022 | C13 | TSA | F | 2 | 50.529 | 2.462 | 87.170 | 1.00 | 28.28 |
| HETATM 6023 | C14 | TSA | F | 2 | 50.208 | 4.019 | 93.994 | 1.00 | 28.83 |
| HETATM 6024 | C15 | TSA | F | 2 | 48.013 | 3.270 | 90.863 | 1.00 | 26.16 |
| HETATM 6025 | C17 | TSA | F | 2 | 47.699 | 12.456 | 93.883 | 1.00 | 27.37 |
| HETATM 6026 | C16 | TSA | F | 2 | 45.610 | 11.107 | 93.679 | 1.00 | 25.36 |
| HETATM 6027 | OH2 | WAT | G | 1 | 61.391 | 6.723 | 88.062 | 1.00 | 12.93 |
| HETATM 6028 | OH2 | WAT | G | 2 | 55.595 | -4.443 | 83.558 | 1.00 | 7.53 |
| HETATM 6029 | OH2 | WAT | G | 3 | 58.656 | 12.731 | 106.749 | 1.00 | 12.33 |
| HETATM 6030 | OH2 | WAT | G | 4 | 46.347 | 15.263 | 111.460 | 1.00 | 14.54 |
| HETATM 6031 | OH2 | WAT | G | 5 | 45.523 | 13.627 | 76.224 | 1.00 | 11.14 |
| HETATM 6032 | OH2 | WAT | G | 6 | 24.466 | -6.064 | 85.688 | 1.00 | 22.41 |
| HETATM 6033 | OH2 | WAT | G | 7 | 48.579 | -17.745 | 80.769 | 1.00 | 21.99 |
| HETATM 6034 | OH2 | WAT | G | 8 | 56.344 | -15.640 | 87.809 | 1.00 | 26.67 |
| HETATM 6035 | OH2 | WAT | G | 9 | 48.554 | -14.901 | 83.717 | 1.00 | 23.94 |
| HETATM 6036 | OH2 | WAT | G | 10 | 57.540 | -7.620 | 122.771 | 1.00 | 26.96 |
| HETATM 6037 | OH2 | WAT | G | 11 | 59.414 | -2.497 | 84.029 | 1.00 | 22.51 |
| HETATM 6038 | OH2 | WAT | G | 12 | 31.671 | 18.074 | 114.616 | 1.00 | 32.15 |
| HETATM 6039 | OH2 | WAT | G | 13 | 62.335 | 10.679 | 117.140 | 1.00 | 19.47 |
| HETATM 6040 | OH2 | WAT | G | 14 | 45.565 | 9.469 | 79.366 | 1.00 | 18.81 |
| HETATM 6041 | OH2 | WAT | G | 15 | 43.311 | 8.237 | 79.508 | 1.00 | 26.11 |
| HETATM 6042 | OH2 | WAT | G | 16 | 46.628 | 13.883 | 104.423 | 1.00 | 24.28 |
| HETATM 6043 | OH2 | WAT | G | 17 | 40.672 | 2.507 | 81.576 | 1.00 | 18.30 |
| HETATM 6044 | OH2 | WAT | G | 18 | 61.830 | 10.923 | 77.709 | 1.00 | 22.27 |
| HETATM 6045 | OH2 | WAT | G | 19 | 57.813 | 0.831 | 108.580 | 1.00 | 24.68 |
| HETATM 6046 | OH2 | WAT | G | 20 | 48.885 | 5.660 | 77.823 | 1.00 | 30.00 |
| HETATM 6047 | OH2 | WAT | G | 21 | 36.382 | -8.352 | 88.841 | 1.00 | 17.32 |
| HETATM 6048 | OH2 | WAT | G | 22 | 39.316 | -10.091 | 86.422 | 1.00 | 27.38 |
| HETATM 6049 | OH2 | WAT | G | 23 | 54.802 | -3.446 | 90.346 | 1.00 | 21.73 |
| HETATM 6050 | OH2 | WAT | G | 24 | 49.292 | 12.112 | 140.537 | 1.00 | 34.17 |
| HETATM 6051 | OH2 | WAT | G | 25 | 56.747 | 8.830 | 60.744 | 1.00 | 40.67 |
| HETATM 6052 | OH2 | WAT | G | 26 | 41.952 | 9.79 | 100.118 | 1.00 | 27.92 |
| HETATM 6053 | OH2 | WAT | G | 27 | 31.268 | 2.80 | 106.695 | 1.00 | 24.31 |
| HETATM 6054 | OH2 | WAT | G | 28 | 68.342 | 17.79 | 111.076 | 1.00 | 30.93 |
| HETATM 6055 | OH2 | WAT | G | 29 | 72.651 | -6.985 | 94.845 | 1.00 | 29.34 |
| HETATM 6056 | OH2 | WAT | G | 30 | 39.287 | 9.257 | 85.623 | 1.00 | 22.61 |
| HETATM 6057 | OH2 | WAT | G | 31 | 61.221 | 14.462 | 87.256 | 1.00 | 29.85 |
| HETATM 6058 | OH2 | WAT | G | 32 | 38.167 | 22.692 | 107.435 | 1.00 | 36.40 |
| HETATM 6059 | OH2 | WAT | G | 33 | 64.657 | -2.682 | 96.225 | 1.00 | 18.70 |
| HETATM 6060 | OH2 | WAT | G | 34 | 44.059 | -2.698 | 99.805 | 1.00 | 30.02 |
| HETATM 6061 | OH2 | WAT | G | 35 | 38.480 | 4.763 | 93.051 | 1.00 | 28.03 |
| HETATM 6062 | OH2 | WAT | G | 36 | 57.899 | 7.654 | 112.976 | 1.00 | 26.46 |
| HETATM 6063 | OH2 | WAT | G | 37 | 57.092 | 3.145 | 93.309 | 1.00 | 22.31 |
| HETATM 6064 | OH2 | WAT | G | 38 | 52.194 | -1.400 | 118.878 | 1.00 | 30.83 |
| HETATM 6065 | OH2 | WAT | G | 39 | 69.400 | 14.200 | 123.379 | 1.00 | 30.98 |
| HETATM 6066 | OH2 | WAT | G | 40 | 24.024 | 6.540 | 79.852 | 1.00 | 38.13 |
| HETATM 6067 | OH2 | WAT | G | 41 | 46.657 | -10.880 | 89.402 | 1.00 | 29.24 |
| HETATM 6068 | OH2 | WAT | G | 42 | 24.976 | 13.489 | 109.692 | 1.00 | 46.34 |
| HETATM 6069 | OH2 | WAT | G | 43 | 46.533 | -4.511 | 94.759 | 1.00 | 23.11 |
| HETATM 6070 | OH2 | WAT | G | 44 | 51.448 | 13.833 | 86.306 | 1.00 | 27.08 |
| HETATM 6071 | OH2 | WAT | G | 45 | 70.578 | 4.183 | 105.248 | 1.00 | 42.42 |
| HETATM 6072 | OH2 | WAT | G | 46 | 53.938 | -9.936 | 116.021 | 1.00 | 38.97 |

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Figure 18-93

| | | | | | | | | | | |
|--------|------|-----|-----|---|-----|--------|---------|---------|------|-------|
| HETATM | 6073 | OH2 | WAT | G | 47 | 38.458 | -0.443 | 63.035 | 1.00 | 28.35 |
| HETATM | 6074 | OH2 | WAT | G | 48 | 64.786 | 7.930 | 107.466 | 1.00 | 34.46 |
| HETATM | 6075 | OH2 | WAT | G | 49 | 50.823 | 36.521 | 114.809 | 1.00 | 40.51 |
| HETATM | 6076 | OH2 | WAT | G | 50 | 33.963 | -10.352 | 68.080 | 1.00 | 39.11 |
| HETATM | 6077 | OH2 | WAT | G | 51 | 71.328 | -14.321 | 86.007 | 1.00 | 33.30 |
| HETATM | 6078 | OH2 | WAT | G | 52 | 63.272 | 10.210 | 79.836 | 1.00 | 35.75 |
| HETATM | 6079 | OH2 | WAT | G | 53 | 59.263 | -12.096 | 94.306 | 1.00 | 29.57 |
| HETATM | 6080 | OH2 | WAT | G | 54 | 46.041 | 10.641 | 76.561 | 1.00 | 27.97 |
| HETATM | 6081 | OH2 | WAT | G | 55 | 46.614 | -13.620 | 89.775 | 1.00 | 24.25 |
| HETATM | 6082 | OH2 | WAT | G | 56 | 76.600 | 0.622 | 89.097 | 1.00 | 29.19 |
| HETATM | 6083 | OH2 | WAT | G | 57 | 53.555 | 6.439 | 79.089 | 1.00 | 34.05 |
| HETATM | 6084 | OH2 | WAT | G | 58 | 71.301 | 11.026 | 83.310 | 1.00 | 35.02 |
| HETATM | 6085 | OH2 | WAT | G | 59 | 28.188 | -9.956 | 81.594 | 1.00 | 33.21 |
| HETATM | 6086 | OH2 | WAT | G | 60 | 53.084 | 20.992 | 98.483 | 1.00 | 27.64 |
| HETATM | 6087 | OH2 | WAT | G | 61 | 59.484 | 8.630 | 93.423 | 1.00 | 30.30 |
| HETATM | 6088 | OH2 | WAT | G | 62 | 26.195 | -3.809 | 95.805 | 1.00 | 33.04 |
| HETATM | 6089 | OH2 | WAT | G | 63 | 26.095 | -0.121 | 89.620 | 1.00 | 37.39 |
| HETATM | 6090 | OH2 | WAT | G | 64 | 47.100 | -6.141 | 109.711 | 1.00 | 20.88 |
| HETATM | 6091 | OH2 | WAT | G | 65 | 23.273 | 0.731 | 92.275 | 1.00 | 30.38 |
| HETATM | 6092 | OH2 | WAT | G | 66 | 45.340 | -24.751 | 72.694 | 1.00 | 37.51 |
| HETATM | 6093 | OH2 | WAT | G | 67 | 33.754 | 16.234 | 111.676 | 1.00 | 34.63 |
| HETATM | 6094 | OH2 | WAT | G | 68 | 52.831 | 19.209 | 126.276 | 1.00 | 47.11 |
| HETATM | 6095 | OH2 | WAT | G | 69 | 50.218 | 16.953 | 111.099 | 1.00 | 26.24 |
| HETATM | 6096 | OH2 | WAT | G | 70 | 44.791 | 5.844 | 70.857 | 1.00 | 24.95 |
| HETATM | 6097 | OH2 | WAT | G | 71 | 49.517 | -18.731 | 82.921 | 1.00 | 29.48 |
| HETATM | 6098 | OH2 | WAT | G | 72 | 76.379 | 10.131 | 116.550 | 1.00 | 48.70 |
| HETATM | 6099 | OH2 | WAT | G | 73 | 30.214 | -8.086 | 87.873 | 1.00 | 46.35 |
| HETATM | 6100 | OH2 | WAT | G | 74 | 45.320 | 12.061 | 80.458 | 1.00 | 30.80 |
| HETATM | 6101 | OH2 | WAT | G | 75 | 72.881 | 5.360 | 86.249 | 1.00 | 29.04 |
| HETATM | 6102 | OH2 | WAT | G | 76 | 59.674 | -23.046 | 87.252 | 1.00 | 41.96 |
| HETATM | 6103 | OH2 | WAT | G | 77 | 40.619 | 7.921 | 100.345 | 1.00 | 26.45 |
| HETATM | 6104 | OH2 | WAT | G | 78 | 41.666 | -19.477 | 70.073 | 1.00 | 36.27 |
| HETATM | 6105 | OH2 | WAT | G | 79 | 46.408 | -6.539 | 92.717 | 1.00 | 25.78 |
| HETATM | 6106 | OH2 | WAT | G | 80 | 35.743 | -12.230 | 81.646 | 1.00 | 28.34 |
| HETATM | 6107 | OH2 | WAT | G | 81 | 28.268 | 8.745 | 121.961 | 1.00 | 41.15 |
| HETATM | 6108 | OH2 | WAT | G | 82 | 68.843 | 3.154 | 71.986 | 1.00 | 32.34 |
| HETATM | 6109 | OH2 | WAT | G | 83 | 52.125 | -11.158 | 85.150 | 1.00 | 24.14 |
| HETATM | 6110 | OH2 | WAT | G | 84 | 75.374 | -1.773 | 92.264 | 1.00 | 26.12 |
| HETATM | 6111 | OH2 | WAT | G | 85 | 46.957 | 12.230 | 142.271 | 1.00 | 37.07 |
| HETATM | 6112 | OH2 | WAT | G | 86 | 63.789 | 9.551 | 64.329 | 1.00 | 55.58 |
| HETATM | 6113 | OH2 | WAT | G | 87 | 60.672 | 21.185 | 72.215 | 1.00 | 58.55 |
| HETATM | 6114 | OH2 | WAT | G | 88 | 56.547 | 9.505 | 82.064 | 1.00 | 31.10 |
| HETATM | 6115 | OH2 | WAT | G | 89 | 26.366 | -0.876 | 92.250 | 1.00 | 29.70 |
| HETATM | 6116 | OH2 | WAT | G | 90 | 67.604 | -16.583 | 80.808 | 1.00 | 32.85 |
| HETATM | 6117 | OH2 | WAT | G | 91 | 23.910 | 1.899 | 82.068 | 1.00 | 42.95 |
| HETATM | 6118 | OH2 | WAT | G | 92 | 50.032 | 4.106 | 117.380 | 1.00 | 30.05 |
| HETATM | 6119 | OH2 | WAT | G | 93 | 26.774 | -9.492 | 83.952 | 1.00 | 43.59 |
| HETATM | 6120 | OH2 | WAT | G | 94 | 42.714 | -0.637 | 113.787 | 1.00 | 40.17 |
| HETATM | 6121 | OH2 | WAT | G | 95 | 57.966 | 7.989 | 134.170 | 1.00 | 47.82 |
| HETATM | 6122 | OH2 | WAT | G | 96 | 54.478 | -3.550 | 119.086 | 1.00 | 36.62 |
| HETATM | 6123 | OH2 | WAT | G | 97 | 53.065 | 11.696 | 101.718 | 1.00 | 41.62 |
| HETATM | 6124 | OH2 | WAT | G | 98 | 58.286 | -23.645 | 68.207 | 1.00 | 45.98 |
| HETATM | 6125 | OH2 | WAT | G | 99 | 54.855 | -9.614 | 121.975 | 1.00 | 34.57 |
| HETATM | 6126 | OH2 | WAT | G | 100 | 57.408 | -3.352 | 57.145 | 1.00 | 42.14 |
| HETATM | 6127 | OH2 | WAT | G | 101 | 63.590 | 20.353 | 123.667 | 1.00 | 33.87 |
| HETATM | 6128 | OH2 | WAT | G | 102 | 48.129 | -23.143 | 72.392 | 1.00 | 30.23 |
| HETATM | 6129 | OH2 | WAT | G | 103 | 62.834 | 6.913 | 76.094 | 1.00 | 52.01 |
| HETATM | 6130 | OH2 | WAT | G | 104 | 34.566 | 6.529 | 73.089 | 1.00 | 36.29 |
| HETATM | 6131 | OH2 | WAT | G | 105 | 51.588 | 20.869 | 67.459 | 1.00 | 36.85 |
| HETATM | 6132 | OH2 | WAT | G | 106 | 28.160 | 18.020 | 129.379 | 1.00 | 42.87 |
| HETATM | 6133 | OH2 | WAT | G | 107 | 49.082 | -11.452 | 57.603 | 1.00 | 43.62 |
| HETATM | 6134 | OH2 | WAT | G | 108 | 44.717 | -8.605 | 93.281 | 1.00 | 41.95 |
| HETATM | 6135 | OH2 | WAT | G | 109 | 67.088 | -11.900 | 94.019 | 1.00 | 35.71 |
| HETATM | 6136 | OH2 | WAT | G | 110 | 49.561 | 22.763 | 100.800 | 1.00 | 35.40 |
| HETATM | 6137 | OH2 | WAT | G | 111 | 75.853 | 10.960 | 124.536 | 1.00 | 56.20 |
| HETATM | 6138 | OH2 | WAT | G | 112 | 54.383 | 8.930 | 136.095 | 1.00 | 36.40 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-94

| | | | | | | |
|-------------|---------------|--------|---------|---------|------|-------|
| HETATM 6139 | OH2 WAT G 113 | 33.114 | 1.764 | 67.443 | 1.00 | 37.01 |
| HETATM 6140 | OH2 WAT G 114 | 42.618 | -4.357 | 102.345 | 1.00 | 39.18 |
| HETATM 6141 | OH2 WAT G 115 | 53.605 | -10.816 | 66.281 | 1.00 | 31.62 |
| HETATM 6142 | OH2 WAT G 116 | 73.410 | -1.010 | 90.400 | 1.00 | 34.72 |
| HETATM 6143 | OH2 WAT G 117 | 68.899 | 3.789 | 110.221 | 1.00 | 35.69 |
| HETATM 6144 | OH2 WAT G 118 | 31.474 | 19.159 | 112.425 | 1.00 | 28.08 |
| HETATM 6145 | OH2 WAT G 119 | 39.749 | -0.616 | 132.457 | 1.00 | 37.43 |
| HETATM 6146 | OH2 WAT G 120 | 44.921 | 1.089 | 137.137 | 1.00 | 40.80 |
| HETATM 6147 | OH2 WAT G 121 | 31.081 | 7.617 | 75.105 | 1.00 | 40.86 |
| HETATM 6148 | OH2 WAT G 122 | 35.554 | 12.017 | 105.965 | 1.00 | 33.58 |
| HETATM 6149 | OH2 WAT G 123 | 41.381 | -23.534 | 70.872 | 1.00 | 38.10 |
| HETATM 6150 | OH2 WAT G 124 | 31.999 | 1.992 | 73.813 | 1.00 | 33.97 |
| HETATM 6151 | OH2 WAT G 125 | 55.761 | 10.285 | 101.654 | 1.00 | 47.66 |
| HETATM 6152 | OH2 WAT G 126 | 30.596 | 12.964 | 133.642 | 1.00 | 37.98 |
| HETATM 6153 | OH2 WAT G 127 | 59.611 | 5.347 | 136.114 | 1.00 | 46.39 |
| HETATM 6154 | OH2 WAT G 128 | 24.190 | 12.220 | 124.679 | 1.00 | 30.77 |
| HETATM 6155 | OH2 WAT G 129 | 70.078 | 4.455 | 86.283 | 1.00 | 36.11 |
| HETATM 6156 | OH2 WAT G 130 | 57.882 | -4.314 | 125.597 | 1.00 | 41.40 |
| HETATM 6157 | OH2 WAT G 131 | 45.838 | -20.690 | 65.884 | 1.00 | 35.98 |
| HETATM 6158 | OH2 WAT G 132 | 47.574 | 3.186 | 79.027 | 1.00 | 36.67 |
| HETATM 6159 | OH2 WAT G 133 | 46.856 | -18.901 | 62.295 | 1.00 | 45.40 |
| HETATM 6160 | OH2 WAT G 134 | 40.164 | 5.047 | 95.358 | 1.00 | 31.38 |
| HETATM 6161 | OH2 WAT G 135 | 27.268 | -0.405 | 122.461 | 1.00 | 38.16 |
| HETATM 6162 | OH2 WAT G 136 | 54.200 | -20.155 | 66.212 | 1.00 | 37.55 |
| HETATM 6163 | OH2 WAT G 137 | 45.435 | -10.534 | 103.626 | 1.00 | 37.96 |
| HETATM 6164 | OH2 WAT G 138 | 31.633 | 25.030 | 106.499 | 1.00 | 43.94 |
| HETATM 6165 | OH2 WAT G 139 | 79.029 | -7.518 | 93.606 | 1.00 | 40.55 |
| HETATM 6166 | OH2 WAT G 140 | 68.597 | 20.711 | 111.685 | 1.00 | 33.25 |
| HETATM 6167 | OH2 WAT G 141 | 64.263 | 8.524 | 113.832 | 1.00 | 40.63 |
| HETATM 6168 | OH2 WAT G 143 | 49.387 | -24.485 | 70.152 | 1.00 | 34.07 |
| HETATM 6169 | OH2 WAT G 144 | 23.383 | -3.854 | 83.604 | 1.00 | 32.22 |
| HETATM 6170 | OH2 WAT G 145 | 42.360 | -0.710 | 61.686 | 1.00 | 35.94 |
| HETATM 6171 | OH2 WAT G 146 | 34.421 | -3.304 | 65.685 | 1.00 | 35.42 |
| HETATM 6172 | OH2 WAT G 147 | 31.506 | 3.409 | 89.579 | 1.00 | 39.86 |
| HETATM 6173 | OH2 WAT G 148 | 34.963 | 10.688 | 91.806 | 1.00 | 31.12 |
| HETATM 6174 | OH2 WAT G 149 | 54.859 | -15.085 | 96.769 | 1.00 | 46.65 |
| HETATM 6175 | OH2 WAT G 150 | 34.695 | 2.391 | 131.273 | 1.00 | 39.22 |
| HETATM 6176 | OH2 WAT G 151 | 40.348 | 1.395 | 61.905 | 1.00 | 34.09 |
| HETATM 6177 | OH2 WAT G 152 | 66.912 | 17.666 | 127.489 | 1.00 | 45.19 |
| HETATM 6178 | OH2 WAT G 153 | 31.096 | 19.900 | 103.232 | 1.00 | 43.45 |
| HETATM 6179 | OH2 WAT G 154 | 28.074 | -4.222 | 70.175 | 1.00 | 28.86 |
| HETATM 6180 | OH2 WAT G 155 | 63.586 | -1.894 | 99.003 | 1.00 | 41.15 |
| HETATM 6181 | OH2 WAT G 156 | 54.145 | -22.222 | 88.415 | 1.00 | 40.92 |
| HETATM 6182 | OH2 WAT G 157 | 62.443 | 13.765 | 89.547 | 1.00 | 33.69 |
| HETATM 6183 | OH2 WAT G 158 | 58.832 | 9.798 | 101.311 | 1.00 | 31.00 |
| HETATM 6184 | OH2 WAT G 159 | 37.701 | -5.528 | 119.322 | 1.00 | 45.00 |
| HETATM 6185 | OH2 WAT G 160 | 43.599 | 13.442 | 131.274 | 1.00 | 38.43 |
| HETATM 6186 | OH2 WAT G 161 | 23.540 | -1.137 | 96.111 | 1.00 | 51.83 |
| HETATM 6187 | OH2 WAT G 162 | 59.915 | -4.318 | 110.873 | 1.00 | 41.92 |
| HETATM 6188 | OH2 WAT G 163 | 51.265 | -8.264 | 60.546 | 1.00 | 31.25 |
| HETATM 6189 | OH2 WAT G 164 | 58.109 | 7.024 | 98.294 | 1.00 | 46.30 |
| HETATM 6190 | OH2 WAT G 165 | 46.553 | 18.195 | 74.179 | 1.00 | 37.53 |
| HETATM 6191 | OH2 WAT G 166 | 55.706 | -21.025 | 92.515 | 1.00 | 43.91 |
| HETATM 6192 | OH2 WAT G 167 | 67.146 | -1.958 | 109.704 | 1.00 | 43.13 |
| HETATM 6193 | OH2 WAT G 168 | 47.445 | -3.047 | 134.746 | 1.00 | 27.99 |
| HETATM 6194 | OH2 WAT G 169 | 65.193 | 5.304 | 63.562 | 1.00 | 36.05 |
| HETATM 6195 | OH2 WAT G 170 | 36.176 | 8.979 | 102.024 | 1.00 | 39.63 |
| HETATM 6196 | OH2 WAT G 171 | 70.527 | 5.797 | 70.886 | 1.00 | 44.69 |
| HETATM 6197 | OH2 WAT G 172 | 67.166 | 8.735 | 74.628 | 1.00 | 51.41 |
| HETATM 6198 | OH2 WAT G 173 | 19.700 | 9.630 | 81.850 | 1.00 | 53.49 |
| HETATM 6199 | OH2 WAT G 174 | 55.875 | 11.277 | 87.176 | 1.00 | 38.63 |
| HETATM 6200 | OH2 WAT G 175 | 61.874 | 8.432 | 91.682 | 1.00 | 40.08 |
| HETATM 6201 | OH2 WAT G 176 | 36.771 | -6.815 | 121.530 | 1.00 | 32.57 |
| HETATM 6202 | OH2 WAT G 177 | 63.224 | 7.776 | 89.317 | 1.00 | 29.83 |
| HETATM 6203 | OH2 WAT G 178 | 29.606 | 15.345 | 132.470 | 1.00 | 47.28 |
| HETATM 6204 | OH2 WAT G 179 | 52.811 | 11.799 | 98.957 | 1.00 | 36.09 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-95

| | | | | | | | | | |
|-------------|-----|-----|---|-----|--------|---------|---------|------|-------|
| HETATM 6205 | OH2 | WAT | G | 180 | 38.589 | 18.249 | 88.356 | 1.00 | 36.19 |
| HETATM 6206 | OH2 | WAT | G | 181 | 43.734 | -15.681 | 61.135 | 1.00 | 34.24 |
| HETATM 6207 | OH2 | WAT | G | 182 | 42.283 | 15.251 | 91.437 | 1.00 | 37.96 |
| HETATM 6208 | OH2 | WAT | G | 183 | 57.121 | -11.129 | 126.206 | 1.00 | 45.78 |
| HETATM 6209 | OH2 | WAT | G | 184 | 50.011 | -19.367 | 92.127 | 1.00 | 36.55 |
| HETATM 6210 | OH2 | WAT | G | 185 | 56.880 | 2.453 | 95.969 | 1.00 | 39.12 |
| HETATM 6211 | OH2 | WAT | G | 186 | 26.356 | 14.125 | 125.052 | 1.00 | 32.68 |
| HETATM 6212 | OH2 | WAT | G | 187 | 24.631 | 20.230 | 122.650 | 1.00 | 45.67 |
| HETATM 6213 | OH2 | WAT | G | 188 | 23.516 | 4.964 | 81.599 | 1.00 | 42.16 |
| HETATM 6214 | OH2 | WAT | G | 189 | 55.017 | 14.964 | 62.948 | 1.00 | 50.18 |
| HETATM 6215 | OH2 | WAT | G | 190 | 33.371 | 13.710 | 105.640 | 1.00 | 37.04 |
| HETATM 6216 | OH2 | WAT | G | 191 | 44.466 | -10.386 | 91.144 | 1.00 | 36.62 |
| HETATM 6217 | OH2 | WAT | G | 192 | 28.437 | 22.668 | 121.285 | 1.00 | 38.19 |
| HETATM 6218 | OH2 | WAT | G | 193 | 29.786 | 24.957 | 122.112 | 1.00 | 42.05 |
| HETATM 6219 | OH2 | WAT | G | 194 | 28.852 | 3.461 | 96.101 | 1.00 | 48.35 |
| HETATM 6220 | OH2 | WAT | G | 195 | 41.681 | 11.318 | 92.011 | 1.00 | 32.60 |
| HETATM 6221 | OH2 | WAT | G | 196 | 26.812 | -10.229 | 111.631 | 1.00 | 47.70 |
| HETATM 6222 | OH2 | WAT | G | 197 | 42.432 | -23.250 | 76.629 | 1.00 | 48.86 |
| HETATM 6223 | OH2 | WAT | G | 198 | 25.484 | 12.756 | 121.410 | 1.00 | 43.09 |
| HETATM 6224 | OH2 | WAT | G | 199 | 43.514 | -20.514 | 111.706 | 1.00 | 46.80 |
| HETATM 6225 | OH2 | WAT | G | 200 | 74.273 | -13.079 | 95.699 | 1.00 | 44.89 |
| HETATM 6226 | OH2 | WAT | G | 201 | 59.982 | 24.381 | 103.984 | 1.00 | 40.63 |
| HETATM 6227 | OH2 | WAT | G | 202 | 67.164 | -12.771 | 74.705 | 1.00 | 35.13 |
| HETATM 6228 | OH2 | WAT | G | 203 | 28.708 | 9.211 | 79.238 | 1.00 | 33.53 |
| HETATM 6229 | OH2 | WAT | G | 204 | 53.256 | -3.576 | 122.243 | 1.00 | 48.49 |
| HETATM 6230 | OH2 | WAT | G | 205 | 50.706 | 16.208 | 87.357 | 1.00 | 41.26 |
| HETATM 6231 | OH2 | WAT | G | 206 | 50.000 | 34.998 | 98.339 | 1.00 | 39.15 |
| HETATM 6232 | OH2 | WAT | G | 207 | 68.078 | -16.236 | 83.621 | 1.00 | 29.70 |
| HETATM 6233 | OH2 | WAT | G | 208 | 24.395 | -4.134 | 111.635 | 1.00 | 50.82 |
| HETATM 6234 | OH2 | WAT | G | 209 | 53.384 | -2.664 | 114.289 | 1.00 | 44.49 |
| HETATM 6235 | OH2 | WAT | G | 210 | 60.120 | -9.482 | 94.788 | 1.00 | 31.97 |
| HETATM 6236 | OH2 | WAT | G | 211 | 23.405 | 17.472 | 111.744 | 1.00 | 44.97 |
| HETATM 6237 | OH2 | WAT | G | 212 | 46.214 | 20.943 | 76.878 | 1.00 | 59.14 |
| HETATM 6238 | OH2 | WAT | G | 213 | 29.754 | 6.983 | 97.109 | 1.00 | 41.78 |
| HETATM 6239 | OH2 | WAT | G | 214 | 46.820 | -0.465 | 55.181 | 1.00 | 41.02 |
| HETATM 6240 | OH2 | WAT | G | 215 | 59.143 | 22.096 | 124.775 | 1.00 | 38.42 |
| HETATM 6241 | OH2 | WAT | G | 216 | 42.674 | 14.088 | 66.037 | 1.00 | 32.50 |
| HETATM 6242 | OH2 | WAT | G | 217 | 55.009 | -7.248 | 98.186 | 1.00 | 56.50 |
| HETATM 6243 | OH2 | WAT | G | 218 | 63.361 | -8.209 | 109.653 | 1.00 | 49.66 |
| HETATM 6244 | OH2 | WAT | G | 219 | 66.583 | -8.146 | 94.671 | 1.00 | 50.91 |
| HETATM 6245 | OH2 | WAT | G | 220 | 44.627 | -2.583 | 93.919 | 1.00 | 36.99 |
| HETATM 6246 | OH2 | WAT | G | 221 | 24.470 | -8.606 | 79.502 | 1.00 | 47.24 |
| HETATM 6247 | OH2 | WAT | G | 222 | 76.913 | -7.777 | 83.973 | 1.00 | 50.43 |
| HETATM 6248 | OH2 | WAT | G | 223 | 32.788 | 0.651 | 129.136 | 1.00 | 42.47 |
| HETATM 6249 | OH2 | WAT | G | 224 | 73.731 | -16.880 | 88.817 | 1.00 | 46.69 |
| HETATM 6250 | OH2 | WAT | G | 225 | 78.567 | -2.802 | 93.970 | 1.00 | 43.17 |
| HETATM 6251 | OH2 | WAT | G | 226 | 45.681 | 1.248 | 57.532 | 1.00 | 35.84 |
| HETATM 6252 | OH2 | WAT | G | 227 | 38.263 | 15.236 | 84.711 | 1.00 | 42.39 |
| HETATM 6253 | OH2 | WAT | G | 228 | 38.933 | 35.224 | 108.488 | 1.00 | 52.23 |
| HETATM 6254 | OH2 | WAT | G | 229 | 33.755 | 14.939 | 70.228 | 1.00 | 46.56 |
| HETATM 6255 | OH2 | WAT | G | 230 | 51.521 | 34.184 | 100.859 | 1.00 | 52.96 |
| HETATM 6256 | OH2 | WAT | G | 231 | 34.140 | 0.565 | 63.039 | 1.00 | 31.02 |
| HETATM 6257 | OH2 | WAT | G | 232 | 37.277 | 13.977 | 81.662 | 1.00 | 39.83 |
| HETATM 6258 | OH2 | WAT | G | 233 | 57.307 | 5.947 | 93.216 | 1.00 | 28.55 |
| HETATM 6259 | OH2 | WAT | G | 234 | 31.718 | 16.820 | 125.707 | 1.00 | 53.16 |
| HETATM 6260 | OH2 | WAT | G | 235 | 60.624 | 31.119 | 110.067 | 1.00 | 51.02 |
| HETATM 6261 | OH2 | WAT | G | 236 | 44.357 | 4.267 | 94.916 | 1.00 | 57.50 |
| HETATM 6262 | OH2 | WAT | G | 237 | 68.454 | 1.072 | 70.111 | 1.00 | 38.65 |
| HETATM 6263 | OH2 | WAT | G | 238 | 27.836 | 6.773 | 79.253 | 1.00 | 44.95 |
| HETATM 6264 | OH2 | WAT | G | 239 | 54.933 | 23.344 | 81.087 | 1.00 | 42.95 |
| HETATM 6265 | OH2 | WAT | G | 240 | 34.072 | -15.271 | 71.579 | 1.00 | 45.78 |
| HETATM 6266 | OH2 | WAT | G | 241 | 35.966 | -1.059 | 61.973 | 1.00 | 38.91 |
| HETATM 6267 | OH2 | WAT | G | 242 | 29.687 | 1.898 | 127.376 | 1.00 | 44.85 |
| HETATM 6268 | OH2 | WAT | G | 243 | 49.534 | -10.150 | 113.501 | 1.00 | 38.32 |
| HETATM 6269 | OH2 | WAT | G | 244 | 57.252 | 9.773 | 96.696 | 1.00 | 48.83 |
| HETATM 6270 | OH2 | WAT | G | 245 | 62.310 | 13.262 | 80.972 | 1.00 | 38.54 |

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Figure 18-96

| | | | | | | |
|-------------|---------------|--------|---------|---------|------|-------|
| HETATM 6271 | OH2 WAT G 246 | 50.248 | -5.552 | 102.815 | 1.00 | 43.23 |
| HETATM 6272 | OH2 WAT G 247 | 47.966 | 21.564 | 79.321 | 1.00 | 36.79 |
| HETATM 6273 | OH2 WAT G 248 | 62.507 | 20.866 | 108.414 | 1.00 | 35.30 |
| HETATM 6274 | OH2 WAT G 249 | 53.971 | 19.763 | 61.067 | 1.00 | 47.49 |
| HETATM 6275 | OH2 WAT G 250 | 38.406 | 9.828 | 67.749 | 1.00 | 33.71 |
| HETATM 6276 | OH2 WAT G 251 | 35.304 | -6.179 | 66.319 | 1.00 | 36.23 |
| HETATM 6277 | OH2 WAT G 252 | 39.218 | -12.667 | 85.010 | 1.00 | 36.17 |
| HETATM 6278 | OH2 WAT G 253 | 56.350 | 5.089 | 97.225 | 1.00 | 46.38 |
| HETATM 6279 | OH2 WAT G 254 | 69.850 | 3.406 | 122.119 | 1.00 | 55.07 |
| HETATM 6280 | OH2 WAT G 255 | 75.703 | 2.630 | 128.600 | 1.00 | 30.64 |
| HETATM 6281 | OH2 WAT G 256 | 32.019 | -12.973 | 113.965 | 1.00 | 34.48 |
| HETATM 6282 | OH2 WAT G 257 | 54.081 | 3.421 | 56.994 | 1.00 | 39.11 |
| HETATM 6283 | OH2 WAT G 258 | 32.801 | -6.170 | 91.078 | 1.00 | 35.72 |
| HETATM 6284 | OH2 WAT G 259 | 45.040 | 0.301 | 95.449 | 1.00 | 36.57 |
| HETATM 6285 | OH2 WAT G 260 | 39.815 | 21.460 | 128.855 | 1.00 | 40.10 |
| HETATM 6286 | OH2 WAT G 261 | 28.763 | 10.408 | 93.790 | 1.00 | 44.39 |
| HETATM 6287 | OH2 WAT G 262 | 49.668 | -12.050 | 60.539 | 1.00 | 50.89 |
| HETATM 6288 | OH2 WAT G 263 | 64.353 | 20.015 | 117.495 | 1.00 | 62.67 |
| HETATM 6289 | OH2 WAT G 264 | 75.183 | 13.021 | 128.124 | 1.00 | 50.42 |
| HETATM 6290 | OH2 WAT G 265 | 46.289 | 6.826 | 52.485 | 1.00 | 46.86 |
| HETATM 6291 | OH2 WAT G 266 | 68.708 | 13.973 | 70.958 | 1.00 | 37.90 |
| HETATM 6292 | OH2 WAT G 267 | 71.504 | 12.997 | 130.029 | 1.00 | 38.78 |
| HETATM 6293 | OH2 WAT G 268 | 36.309 | -4.716 | 130.364 | 1.00 | 42.92 |
| HETATM 6294 | OH2 WAT G 269 | 65.973 | 12.195 | 79.625 | 1.00 | 51.68 |
| HETATM 6295 | OH2 WAT G 270 | 71.952 | 13.021 | 74.292 | 1.00 | 37.70 |
| HETATM 6296 | OH2 WAT G 271 | 44.433 | -17.578 | 62.734 | 1.00 | 49.33 |
| HETATM 6297 | OH2 WAT G 272 | 26.917 | 15.038 | 89.067 | 1.00 | 38.07 |
| HETATM 6298 | OH2 WAT G 273 | 63.380 | -5.416 | 126.550 | 1.00 | 41.73 |
| HETATM 6299 | OH2 WAT G 274 | 63.360 | -5.356 | 95.641 | 1.00 | 37.54 |
| HETATM 6300 | OH2 WAT G 275 | 65.947 | -13.015 | 97.485 | 1.00 | 37.42 |
| HETATM 6301 | OH2 WAT G 276 | 26.406 | 25.831 | 117.328 | 1.00 | 48.37 |
| HETATM 6302 | OH2 WAT G 277 | 41.893 | -10.251 | 98.201 | 1.00 | 46.36 |
| HETATM 6303 | OH2 WAT G 278 | 30.343 | -6.507 | 117.764 | 1.00 | 49.87 |
| HETATM 6304 | OH2 WAT G 279 | 45.135 | 32.419 | 111.056 | 1.00 | 43.93 |
| HETATM 6305 | OH2 WAT G 280 | 50.553 | -1.365 | 120.511 | 1.00 | 54.02 |
| HETATM 6306 | OH2 WAT G 281 | 60.428 | 13.652 | 105.130 | 1.00 | 31.10 |
| HETATM 6307 | OH2 WAT G 282 | 30.342 | 2.204 | 70.246 | 1.00 | 45.19 |
| HETATM 6308 | OH2 WAT G 283 | 60.358 | 15.921 | 127.736 | 1.00 | 33.17 |
| HETATM 6309 | OH2 WAT G 284 | 64.193 | 3.421 | 62.117 | 1.00 | 45.81 |
| HETATM 6310 | OH2 WAT G 285 | 45.468 | 6.113 | 105.853 | 1.00 | 48.98 |
| HETATM 6311 | OH2 WAT G 286 | 47.514 | 3.808 | 98.279 | 1.00 | 46.45 |
| HETATM 6312 | OH2 WAT G 287 | 72.144 | -6.345 | 77.930 | 1.00 | 40.04 |
| HETATM 6313 | OH2 WAT G 288 | 54.142 | -5.100 | 99.674 | 1.00 | 43.62 |
| HETATM 6314 | OH2 WAT G 289 | 48.982 | 13.297 | 65.822 | 1.00 | 46.98 |
| HETATM 6315 | OH2 WAT G 290 | 41.171 | 34.107 | 115.807 | 1.00 | 51.76 |
| HETATM 6316 | OH2 WAT G 291 | 36.494 | 37.195 | 104.170 | 1.00 | 44.27 |
| HETATM 6317 | OH2 WAT G 292 | 48.580 | 23.117 | 85.456 | 1.00 | 40.96 |
| HETATM 6318 | OH2 WAT G 293 | 55.853 | 22.934 | 98.099 | 1.00 | 40.95 |
| HETATM 6319 | OH2 WAT G 294 | 61.720 | 11.077 | 89.427 | 1.00 | 41.21 |
| HETATM 6320 | OH2 WAT G 295 | 43.313 | -18.552 | 114.112 | 1.00 | 42.32 |
| HETATM 6321 | OH2 WAT G 296 | 53.001 | -6.305 | 129.052 | 1.00 | 37.41 |
| HETATM 6322 | OH2 WAT G 297 | 70.258 | 24.928 | 82.843 | 1.00 | 48.09 |
| HETATM 6323 | OH2 WAT G 298 | 77.493 | 0.940 | 130.507 | 1.00 | 51.77 |
| HETATM 6324 | OH2 WAT G 299 | 32.233 | 12.182 | 83.028 | 1.00 | 53.51 |
| HETATM 6325 | OH2 WAT G 300 | 40.666 | 12.878 | 65.747 | 1.00 | 46.49 |
| HETATM 6326 | OH2 WAT G 301 | 50.977 | 12.831 | 114.597 | 1.00 | 48.51 |
| HETATM 6327 | OH2 WAT G 302 | 54.236 | 3.817 | 92.196 | 1.00 | 41.15 |
| HETATM 6328 | OH2 WAT G 303 | 59.527 | -1.343 | 107.471 | 1.00 | 36.71 |
| HETATM 6329 | OH2 WAT G 304 | 70.331 | 3.940 | 89.312 | 1.00 | 47.70 |
| HETATM 6330 | OH2 WAT G 305 | 60.626 | 6.969 | 127.780 | 1.00 | 41.96 |
| HETATM 6331 | OH2 WAT G 306 | 42.156 | -0.139 | 133.156 | 1.00 | 32.19 |
| HETATM 6332 | OH2 WAT G 307 | 58.886 | 16.514 | 99.413 | 1.00 | 53.60 |
| HETATM 6333 | OH2 WAT G 308 | 67.617 | -1.589 | 96.570 | 1.00 | 40.36 |
| HETATM 6334 | OH2 WAT G 309 | 35.868 | -10.936 | 98.849 | 1.00 | 48.80 |
| HETATM 6335 | OH2 WAT G 310 | 45.576 | 25.388 | 131.914 | 1.00 | 48.99 |
| HETATM 6336 | OH2 WAT G 311 | 37.583 | -6.243 | 64.257 | 1.00 | 37.06 |

SUBSTITUTE SHEET (RULE 26)

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Figure 18-97

| | | | | | | | | | | |
|--------|------|-----|-----|---|-----|--------|---------|---------|------|-------|
| HETATM | 6337 | OH2 | WAT | G | 312 | 66.759 | 16.408 | 94.600 | 1.00 | 45.07 |
| HETATM | 6338 | OH2 | WAT | G | 313 | 24.142 | 11.212 | 113.340 | 1.00 | 52.23 |
| HETATM | 6339 | OH2 | WAT | G | 314 | 69.409 | 16.702 | 64.230 | 1.00 | 39.88 |
| HETATM | 6340 | OH2 | WAT | G | 315 | 22.064 | 24.858 | 115.328 | 1.00 | 50.23 |
| HETATM | 6341 | OH2 | WAT | G | 316 | 50.171 | 9.551 | 100.345 | 1.00 | 37.32 |
| HETATM | 6342 | OH2 | WAT | G | 317 | 55.104 | 31.302 | 119.497 | 1.00 | 44.78 |
| HETATM | 6343 | OH2 | WAT | G | 318 | 65.333 | -10.105 | 95.866 | 1.00 | 44.21 |
| HETATM | 6344 | OH2 | WAT | G | 319 | 31.415 | -2.472 | 128.127 | 1.00 | 41.95 |
| HETATM | 6345 | OH2 | WAT | G | 320 | 37.423 | 13.143 | 88.069 | 1.00 | 44.79 |
| HETATM | 6346 | OH2 | WAT | G | 321 | 43.619 | 14.292 | 96.509 | 1.00 | 54.69 |
| HETATM | 6347 | OH2 | WAT | G | 322 | 68.048 | 14.555 | 126.016 | 1.00 | 42.75 |
| HETATM | 6348 | OH2 | WAT | G | 323 | 34.778 | -2.509 | 130.204 | 1.00 | 37.06 |
| HETATM | 6349 | OH2 | WAT | G | 324 | 27.972 | 18.144 | 103.841 | 1.00 | 47.34 |
| HETATM | 6350 | OH2 | WAT | G | 325 | 53.550 | 23.610 | 97.592 | 1.00 | 38.03 |
| HETATM | 6351 | OH2 | WAT | G | 326 | 33.776 | 4.171 | 103.451 | 1.00 | 50.60 |
| HETATM | 6352 | OH2 | WAT | G | 327 | 37.862 | 35.632 | 114.870 | 1.00 | 48.34 |
| HETATM | 6353 | OH2 | WAT | G | 328 | 50.893 | 14.612 | 93.478 | 1.00 | 38.77 |
| HETATM | 6354 | OH2 | WAT | G | 329 | 71.422 | -20.913 | 86.137 | 1.00 | 47.69 |
| HETATM | 6355 | OH2 | WAT | G | 330 | 50.310 | -23.133 | 74.502 | 1.00 | 41.94 |
| HETATM | 6356 | OH2 | WAT | G | 331 | 41.520 | 7.269 | 60.583 | 1.00 | 54.93 |
| HETATM | 6357 | OH2 | WAT | G | 332 | 75.879 | 13.737 | 106.089 | 1.00 | 44.65 |
| HETATM | 6358 | OH2 | WAT | G | 333 | 51.923 | 9.027 | 138.493 | 1.00 | 41.08 |
| HETATM | 6359 | OH2 | WAT | G | 334 | 49.511 | 27.611 | 79.363 | 1.00 | 39.05 |
| HETATM | 6360 | OH2 | WAT | G | 335 | 69.385 | 0.852 | 110.192 | 1.00 | 41.42 |
| HETATM | 6361 | OH2 | WAT | G | 336 | 40.952 | 2.479 | 101.880 | 1.00 | 42.50 |
| HETATM | 6362 | OH2 | WAT | G | 337 | 32.998 | 7.200 | 103.784 | 1.00 | 54.22 |
| HETATM | 6363 | OH2 | WAT | G | 338 | 54.366 | 15.261 | 136.205 | 1.00 | 52.69 |
| HETATM | 6364 | OH2 | WAT | G | 339 | 35.674 | 13.727 | 89.792 | 1.00 | 35.83 |
| HETATM | 6365 | OH2 | WAT | G | 340 | 66.606 | -21.361 | 87.138 | 1.00 | 46.26 |
| HETATM | 6366 | OH2 | WAT | G | 341 | 72.053 | 4.708 | 131.550 | 1.00 | 45.27 |
| HETATM | 6367 | OH2 | WAT | G | 342 | 28.072 | -1.358 | 70.419 | 1.00 | 34.92 |
| HETATM | 6368 | OH2 | WAT | G | 343 | 23.611 | -3.981 | 76.422 | 1.00 | 52.39 |
| HETATM | 6369 | OH2 | WAT | G | 344 | 53.684 | 2.564 | 122.150 | 1.00 | 58.16 |
| HETATM | 6370 | OH2 | WAT | G | 345 | 30.624 | -6.528 | 125.556 | 1.00 | 34.71 |
| HETATM | 6371 | OH2 | WAT | G | 346 | 27.870 | 13.838 | 113.997 | 1.00 | 44.91 |
| HETATM | 6372 | OH2 | WAT | G | 347 | 31.903 | -9.588 | 116.327 | 1.00 | 55.34 |
| HETATM | 6373 | OH2 | WAT | G | 348 | 71.763 | 15.094 | 63.739 | 1.00 | 48.99 |
| HETATM | 6374 | OH2 | WAT | G | 349 | 25.258 | -2.536 | 114.760 | 1.00 | 37.19 |
| HETATM | 6375 | OH2 | WAT | G | 350 | 43.765 | 12.162 | 78.143 | 1.00 | 42.32 |
| HETATM | 6376 | OH2 | WAT | G | 351 | 32.452 | 5.338 | 73.909 | 1.00 | 33.70 |
| HETATM | 6377 | OH2 | WAT | G | 352 | 52.896 | -5.770 | 101.894 | 1.00 | 46.40 |
| HETATM | 6378 | OH2 | WAT | G | 353 | 47.968 | 4.242 | 115.852 | 1.00 | 34.62 |
| HETATM | 6379 | OH2 | WAT | G | 354 | 38.561 | -9.302 | 90.596 | 1.00 | 49.80 |
| HETATM | 6380 | OH2 | WAT | G | 355 | 63.791 | 17.454 | 74.354 | 1.00 | 56.40 |
| HETATM | 6381 | OH2 | WAT | G | 356 | 41.360 | 2.648 | 133.760 | 1.00 | 50.00 |
| HETATM | 6382 | OH2 | WAT | G | 357 | 42.467 | -7.937 | 122.328 | 1.00 | 38.01 |
| HETATM | 6383 | OH2 | WAT | G | 358 | 50.890 | -0.362 | 116.668 | 1.00 | 39.26 |
| HETATM | 6384 | OH2 | WAT | G | 359 | 54.217 | -23.881 | 67.865 | 1.00 | 55.18 |
| HETATM | 6385 | OH2 | WAT | G | 360 | 64.959 | 9.539 | 105.032 | 1.00 | 38.83 |
| HETATM | 6386 | OH2 | WAT | G | 361 | 58.113 | -19.846 | 82.288 | 1.00 | 38.60 |
| HETATM | 6387 | OH2 | WAT | G | 362 | 42.245 | -1.140 | 93.572 | 1.00 | 31.47 |
| HETATM | 6388 | OH2 | WAT | G | 363 | 73.552 | 17.770 | 125.885 | 1.00 | 54.89 |
| HETATM | 6389 | OH2 | WAT | G | 364 | 68.769 | 15.898 | 106.810 | 1.00 | 45.53 |
| HETATM | 6390 | OH2 | WAT | G | 365 | 37.543 | 19.031 | 78.866 | 1.00 | 45.15 |
| HETATM | 6391 | OH2 | WAT | G | 366 | 55.583 | 6.906 | 95.087 | 1.00 | 44.99 |
| HETATM | 6392 | OH2 | WAT | G | 367 | 41.284 | 9.699 | 78.250 | 1.00 | 36.58 |
| HETATM | 6393 | OH2 | WAT | G | 368 | 25.203 | 5.332 | 126.362 | 1.00 | 46.60 |
| HETATM | 6394 | OH2 | WAT | G | 369 | 74.742 | -5.006 | 95.104 | 1.00 | 47.85 |
| HETATM | 6395 | OH2 | WAT | G | 370 | 70.349 | 19.871 | 69.925 | 1.00 | 51.46 |
| HETATM | 6396 | OH2 | WAT | G | 371 | 42.936 | 20.631 | 94.720 | 1.00 | 38.66 |
| HETATM | 6397 | OH2 | WAT | G | 372 | 34.162 | -16.114 | 114.141 | 1.00 | 44.01 |
| HETATM | 6398 | OH2 | WAT | G | 373 | 33.863 | 16.838 | 100.275 | 1.00 | 44.66 |
| HETATM | 6399 | OH2 | WAT | G | 374 | 21.613 | 12.569 | 86.140 | 1.00 | 43.89 |
| HETATM | 6400 | OH2 | WAT | G | 375 | 35.751 | -13.302 | 100.583 | 1.00 | 53.53 |
| HETATM | 6401 | OH2 | WAT | G | 376 | 70.095 | 13.395 | 117.505 | 1.00 | 52.02 |
| HETATM | 6402 | OH2 | WAT | G | 377 | 41.853 | 19.108 | 131.799 | 1.00 | 46.47 |

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Figure 18-98

| | | | | | | |
|-------------|---------------|--------|---------|---------|------|-------|
| HETATM 6403 | OH2 WAT G 378 | 55.780 | -14.986 | 65.487 | 1.00 | 49.09 |
| HETATM 6404 | OH2 WAT G 379 | 40.990 | 21.205 | 91.611 | 1.00 | 41.02 |
| HETATM 6405 | OH2 WAT G 380 | 48.157 | 1.057 | 116.992 | 1.00 | 44.84 |
| HETATM 6406 | OH2 WAT G 381 | 37.954 | -6.221 | 128.334 | 1.00 | 37.09 |
| HETATM 6407 | OH2 WAT G 382 | 30.221 | 27.743 | 109.194 | 1.00 | 39.92 |
| HETATM 6408 | OH2 WAT G 383 | 49.926 | -12.826 | 118.421 | 1.00 | 58.95 |
| HETATM 6409 | OH2 WAT G 384 | 42.435 | -17.636 | 81.477 | 1.00 | 48.47 |
| HETATM 6410 | OH2 WAT G 385 | 58.226 | -25.990 | 71.378 | 1.00 | 48.18 |
| HETATM 6411 | OH2 WAT G 386 | 40.495 | 17.944 | 128.741 | 1.00 | 43.82 |
| HETATM 6412 | OH2 WAT G 387 | 31.943 | 6.301 | 109.475 | 1.00 | 35.53 |
| HETATM 6413 | OH2 WAT G 388 | 47.277 | 2.559 | 100.509 | 1.00 | 43.00 |
| HETATM 6414 | OH2 WAT G 389 | 38.862 | 9.112 | 102.620 | 1.00 | 31.70 |
| HETATM 6415 | OH2 WAT G 390 | 71.652 | 14.568 | 105.167 | 1.00 | 49.63 |
| HETATM 6416 | OH2 WAT G 391 | 68.554 | -10.518 | 73.331 | 1.00 | 38.16 |
| HETATM 6417 | OH2 WAT G 392 | 70.496 | -16.160 | 84.425 | 1.00 | 32.16 |
| HETATM 6418 | OH2 WAT G 393 | 44.698 | -24.950 | 75.603 | 1.00 | 43.38 |
| HETATM 6419 | OH2 WAT G 394 | 56.172 | 15.369 | 55.027 | 1.00 | 47.44 |
| HETATM 6420 | OH2 WAT G 395 | 46.150 | -9.441 | 99.999 | 1.00 | 47.98 |
| HETATM 6421 | OH2 WAT G 396 | 26.892 | -8.356 | 89.057 | 1.00 | 34.99 |
| HETATM 6422 | OH2 WAT G 397 | 31.737 | 14.380 | 90.395 | 1.00 | 50.78 |
| HETATM 6423 | OH2 WAT G 398 | 36.261 | -13.824 | 62.777 | 1.00 | 50.86 |
| HETATM 6424 | OH2 WAT G 399 | 37.312 | 15.242 | 134.977 | 1.00 | 43.57 |
| HETATM 6425 | OH2 WAT G 400 | 33.728 | 13.773 | 126.419 | 1.00 | 57.13 |
| HETATM 6426 | OH2 WAT G 401 | 45.269 | 27.937 | 130.311 | 1.00 | 49.55 |
| HETATM 6427 | OH2 WAT G 402 | 44.887 | -17.414 | 111.508 | 1.00 | 54.29 |
| HETATM 6428 | OH2 WAT G 403 | 68.928 | 0.455 | 136.711 | 1.00 | 49.90 |
| HETATM 6429 | OH2 WAT G 404 | 43.271 | -21.571 | 64.425 | 1.00 | 48.61 |
| HETATM 6430 | OH2 WAT G 405 | 24.243 | -4.781 | 108.590 | 1.00 | 51.05 |
| HETATM 6431 | OH2 WAT G 406 | 54.828 | 5.311 | 59.009 | 1.00 | 43.43 |
| HETATM 6432 | OH2 WAT G 407 | 53.460 | 27.992 | 124.076 | 1.00 | 47.83 |
| HETATM 6433 | OH2 WAT G 408 | 70.833 | -18.390 | 85.386 | 1.00 | 49.26 |
| HETATM 6434 | OH2 WAT G 409 | 71.497 | 15.287 | 113.071 | 1.00 | 34.52 |
| HETATM 6435 | OH2 WAT G 410 | 36.407 | -18.480 | 110.466 | 1.00 | 55.43 |
| HETATM 6436 | OH2 WAT G 411 | 26.220 | -9.551 | 78.158 | 1.00 | 47.69 |
| HETATM 6437 | OH2 WAT G 412 | 52.319 | 26.326 | 82.038 | 1.00 | 42.00 |
| HETATM 6438 | OH2 WAT G 413 | 76.173 | 14.097 | 122.253 | 1.00 | 44.90 |
| HETATM 6439 | OH2 WAT G 414 | 58.379 | 6.335 | 123.024 | 1.00 | 54.61 |
| HETATM 6440 | OH2 WAT G 415 | 72.162 | -16.705 | 82.719 | 1.00 | 50.63 |
| HETATM 6441 | OH2 WAT G 416 | 63.557 | 26.152 | 65.944 | 1.00 | 39.83 |
| HETATM 6442 | OH2 WAT G 417 | 38.935 | 23.070 | 122.742 | 1.00 | 52.57 |
| HETATM 6443 | OH2 WAT G 418 | 55.256 | -10.714 | 124.501 | 1.00 | 42.38 |
| HETATM 6444 | OH2 WAT G 419 | 55.443 | -9.037 | 110.170 | 1.00 | 46.47 |
| HETATM 6445 | OH2 WAT G 420 | 73.873 | 16.578 | 123.288 | 1.00 | 46.54 |
| HETATM 6446 | OH2 WAT G 421 | 74.426 | 12.663 | 117.527 | 1.00 | 43.62 |
| HETATM 6447 | OH2 WAT G 422 | 52.374 | -0.368 | 51.502 | 1.00 | 56.99 |
| HETATM 6448 | OH2 WAT G 423 | 60.339 | 20.215 | 84.713 | 1.00 | 36.27 |
| HETATM 6449 | OH2 WAT G 424 | 48.308 | 1.354 | 54.561 | 1.00 | 38.53 |
| HETATM 6450 | OH2 WAT G 425 | 61.757 | 21.606 | 115.976 | 1.00 | 61.09 |
| HETATM 6451 | OH2 WAT G 426 | 33.222 | -14.916 | 119.528 | 1.00 | 51.12 |
| HETATM 6452 | OH2 WAT G 427 | 47.477 | 3.359 | 112.298 | 1.00 | 46.10 |
| HETATM 6453 | OH2 WAT G 428 | 39.909 | 2.272 | 138.388 | 1.00 | 35.33 |
| HETATM 6454 | OH2 WAT G 429 | 57.829 | 15.336 | 126.262 | 1.00 | 62.59 |
| HETATM 6455 | OH2 WAT G 430 | 48.917 | -5.857 | 119.191 | 1.00 | 51.45 |
| HETATM 6456 | OH2 WAT G 431 | 44.139 | -3.812 | 132.964 | 1.00 | 44.91 |
| HETATM 6457 | OH2 WAT G 432 | 38.885 | 18.594 | 95.398 | 1.00 | 50.23 |
| HETATM 6458 | OH2 WAT G 433 | 52.628 | -7.064 | 55.271 | 1.00 | 39.96 |
| HETATM 6459 | OH2 WAT G 434 | 60.644 | -0.731 | 101.129 | 1.00 | 47.30 |
| HETATM 6460 | OH2 WAT G 435 | 64.772 | 5.808 | 71.942 | 1.00 | 50.81 |
| HETATM 6461 | OH2 WAT G 436 | 39.571 | 16.705 | 80.180 | 1.00 | 34.07 |
| HETATM 6462 | OH2 WAT G 437 | 32.791 | -0.551 | 65.371 | 1.00 | 41.40 |
| HETATM 6463 | OH2 WAT G 438 | 58.318 | -7.989 | 60.087 | 1.00 | 46.94 |
| HETATM 6464 | OH2 WAT G 439 | 26.982 | 5.474 | 120.408 | 1.00 | 46.28 |
| HETATM 6465 | OH2 WAT G 440 | 72.138 | 1.233 | 90.050 | 1.00 | 50.13 |
| HETATM 6466 | OH2 WAT G 441 | 29.494 | 10.971 | 118.393 | 1.00 | 56.30 |
| HETATM 6467 | OH2 WAT G 442 | 69.232 | 5.594 | 113.941 | 1.00 | 58.17 |
| HETATM 6468 | OH2 WAT G 443 | 61.459 | 11.576 | 71.140 | 1.00 | 61.67 |

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Figure 18-99

| | | | | | | | | | | |
|--------|------|-----|-----|---|-----|--------|---------|---------|------|-------|
| HETATM | 6469 | OH2 | WAT | G | 444 | 59.592 | 2.195 | 58.518 | 1.00 | 42.66 |
| HETATM | 6470 | OH2 | WAT | G | 445 | 47.407 | 6.152 | 111.310 | 1.00 | 45.14 |
| HETATM | 6471 | OH2 | WAT | G | 446 | 36.254 | 18.203 | 99.930 | 1.00 | 44.76 |
| HETATM | 6472 | OH2 | WAT | G | 447 | 49.525 | 32.050 | 116.235 | 1.00 | 47.72 |
| HETATM | 6473 | OH2 | WAT | G | 448 | 21.801 | -5.358 | 81.109 | 1.00 | 42.07 |
| HETATM | 6474 | OH2 | WAT | G | 449 | 52.131 | -14.007 | 95.380 | 1.00 | 40.76 |
| HETATM | 6475 | OH2 | WAT | G | 450 | 39.712 | -19.983 | 72.499 | 1.00 | 51.69 |
| HETATM | 6476 | OH2 | WAT | G | 451 | 67.651 | 5.620 | 67.102 | 1.00 | 42.38 |
| HETATM | 6477 | OH2 | WAT | G | 452 | 77.344 | 1.313 | 79.207 | 1.00 | 63.64 |
| HETATM | 6478 | OH2 | WAT | G | 453 | 55.249 | -29.426 | 86.187 | 1.00 | 44.98 |
| HETATM | 6479 | OH2 | WAT | G | 454 | 64.429 | -11.004 | 98.104 | 1.00 | 49.12 |
| HETATM | 6480 | OH2 | WAT | G | 455 | 45.456 | -0.814 | 129.510 | 1.00 | 61.60 |
| HETATM | 6481 | OH2 | WAT | G | 456 | 65.066 | -14.790 | 68.028 | 1.00 | 40.08 |
| HETATM | 6482 | OH2 | WAT | G | 457 | 34.732 | 5.611 | 94.924 | 1.00 | 58.32 |

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Figure 19-1

| | | | | Residue # | X | Y | Z | B | Segment ID | ID | |
|------|----|-----|-----|-----------|----|--------|--------|--------|------------|-------|------|
| ATOM | 1 | CE | ALA | A | 2 | 45.868 | 37.229 | 75.022 | 1.00 | 57.10 | AAAA |
| ATOM | 2 | C | ALA | A | 2 | 46.761 | 38.761 | 73.244 | 1.00 | 55.49 | AAAA |
| ATOM | 3 | O | ALA | A | 2 | 46.339 | 39.800 | 73.750 | 1.00 | 55.57 | AAAA |
| ATOM | 4 | N | ALA | A | 2 | 48.280 | 37.746 | 74.937 | 1.00 | 57.26 | AAAA |
| ATOM | 5 | CA | ALA | A | 2 | 47.062 | 37.537 | 74.110 | 1.00 | 56.37 | AAAA |
| ATOM | 6 | N | LYS | A | 3 | 46.976 | 38.628 | 71.938 | 1.00 | 53.94 | AAAA |
| ATOM | 7 | CA | LYS | A | 3 | 46.721 | 39.716 | 71.002 | 1.00 | 51.97 | AAAA |
| ATOM | 8 | CB | LYS | A | 3 | 47.815 | 39.778 | 69.939 | 1.00 | 53.86 | AAAA |
| ATOM | 9 | CG | LYS | A | 3 | 49.223 | 39.876 | 70.490 | 1.00 | 56.47 | AAAA |
| ATOM | 10 | CD | LYS | A | 3 | 50.252 | 39.670 | 69.387 | 1.00 | 57.84 | AAAA |
| ATOM | 11 | CE | LYS | A | 3 | 51.654 | 39.597 | 69.957 | 1.00 | 58.89 | AAAA |
| ATOM | 12 | NZ | LYS | A | 3 | 52.643 | 39.283 | 68.895 | 1.00 | 59.83 | AAAA |
| ATOM | 13 | C | LYS | A | 3 | 45.393 | 39.494 | 70.305 | 1.00 | 49.57 | AAAA |
| ATOM | 14 | O | LYS | A | 3 | 44.894 | 38.373 | 70.246 | 1.00 | 49.33 | AAAA |
| ATOM | 15 | N | VAL | A | 4 | 44.826 | 40.574 | 69.777 | 1.00 | 46.23 | AAAA |
| ATOM | 16 | CA | VAL | A | 4 | 43.561 | 40.516 | 69.056 | 1.00 | 42.51 | AAAA |
| ATOM | 17 | CB | VAL | A | 4 | 42.543 | 41.516 | 69.630 | 1.00 | 42.26 | AAAA |
| ATOM | 18 | CG1 | VAL | A | 4 | 41.213 | 41.352 | 68.940 | 1.00 | 41.51 | AAAA |
| ATOM | 19 | CG2 | VAL | A | 4 | 42.401 | 41.307 | 71.128 | 1.00 | 42.00 | AAAA |
| ATOM | 20 | C | VAL | A | 4 | 43.918 | 40.913 | 67.638 | 1.00 | 39.94 | AAAA |
| ATOM | 21 | O | VAL | A | 4 | 44.332 | 42.032 | 67.395 | 1.00 | 40.39 | AAAA |
| ATOM | 22 | N | LYS | A | 5 | 43.766 | 40.001 | 66.695 | 1.00 | 36.94 | AAAA |
| ATOM | 23 | CA | LYS | A | 5 | 44.142 | 40.305 | 65.323 | 1.00 | 34.10 | AAAA |
| ATOM | 24 | CB | LYS | A | 5 | 45.179 | 39.290 | 64.846 | 1.00 | 35.02 | AAAA |
| ATOM | 25 | CG | LYS | A | 5 | 46.424 | 39.182 | 65.698 | 1.00 | 34.07 | AAAA |
| ATOM | 26 | CD | LYS | A | 5 | 47.233 | 40.452 | 65.652 | 1.00 | 33.44 | AAAA |
| ATOM | 27 | CE | LYS | A | 5 | 48.565 | 40.239 | 66.333 | 1.00 | 32.38 | AAAA |
| ATOM | 28 | NZ | LYS | A | 5 | 49.372 | 41.460 | 66.222 | 1.00 | 31.26 | AAAA |
| ATOM | 29 | C | LYS | A | 5 | 42.997 | 40.293 | 64.333 | 1.00 | 31.38 | AAAA |
| ATOM | 30 | O | LYS | A | 5 | 42.053 | 39.523 | 64.466 | 1.00 | 31.74 | AAAA |
| ATOM | 31 | N | LEU | A | 6 | 43.090 | 41.142 | 63.326 | 1.00 | 28.60 | AAAA |
| ATOM | 32 | CA | LEU | A | 6 | 42.075 | 41.167 | 62.289 | 1.00 | 26.90 | AAAA |
| ATOM | 33 | CB | LEU | A | 6 | 41.530 | 42.580 | 62.067 | 1.00 | 26.43 | AAAA |
| ATOM | 34 | CG | LEU | A | 6 | 40.321 | 42.748 | 61.129 | 1.00 | 25.89 | AAAA |
| ATOM | 35 | CD1 | LEU | A | 6 | 40.108 | 44.224 | 60.826 | 1.00 | 25.50 | AAAA |
| ATOM | 36 | CD2 | LEU | A | 6 | 40.550 | 42.032 | 59.828 | 1.00 | 26.64 | AAAA |
| ATOM | 37 | C | LEU | A | 6 | 42.818 | 40.701 | 61.049 | 1.00 | 25.74 | AAAA |
| ATOM | 38 | O | LEU | A | 6 | 43.877 | 41.226 | 60.717 | 1.00 | 24.60 | AAAA |
| ATOM | 39 | N | ILE | A | 7 | 42.282 | 39.704 | 60.357 | 1.00 | 25.90 | AAAA |
| ATOM | 40 | CA | ILE | A | 7 | 42.939 | 39.212 | 59.173 | 1.00 | 26.75 | AAAA |
| ATOM | 41 | CB | ILE | A | 7 | 42.839 | 37.712 | 59.089 | 1.00 | 26.58 | AAAA |
| ATOM | 42 | CG2 | ILE | A | 7 | 43.474 | 37.227 | 57.783 | 1.00 | 27.88 | AAAA |
| ATOM | 43 | CG1 | ILE | A | 7 | 43.528 | 37.116 | 60.310 | 1.00 | 27.02 | AAAA |
| ATOM | 44 | CD1 | ILE | A | 7 | 43.507 | 35.640 | 60.350 | 1.00 | 27.46 | AAAA |
| ATOM | 45 | C | ILE | A | 7 | 42.339 | 39.814 | 57.929 | 1.00 | 26.70 | AAAA |
| ATOM | 46 | O | ILE | A | 7 | 41.162 | 39.655 | 57.681 | 1.00 | 27.68 | AAAA |
| ATOM | 47 | N | GLY | A | 8 | 43.144 | 40.509 | 57.142 | 1.00 | 27.94 | AA A |
| ATOM | 48 | CA | GLY | A | 8 | 42.598 | 41.110 | 55.944 | 1.00 | 29.78 | AA A |
| ATOM | 49 | C | GLY | A | 8 | 43.587 | 41.789 | 55.027 | 1.00 | 30.38 | AAAA |
| ATOM | 50 | O | GLY | A | 8 | 44.785 | 41.765 | 55.264 | 1.00 | 29.39 | AAAA |
| ATOM | 51 | N | THR | A | 9 | 43.051 | 42.395 | 53.971 | 1.00 | 31.84 | AAAA |
| ATOM | 52 | CA | THR | A | 9 | 43.832 | 43.106 | 52.962 | 1.00 | 32.41 | AAAA |
| ATOM | 53 | CB | THR | A | 9 | 44.606 | 42.112 | 52.064 | 1.00 | 31.12 | AAAA |
| ATOM | 54 | CG1 | THR | A | 9 | 45.324 | 42.825 | 51.053 | 1.00 | 30.74 | AAAA |
| ATOM | 55 | CG2 | THR | A | 9 | 43.654 | 41.140 | 51.411 | 1.00 | 30.27 | AAAA |
| ATOM | 56 | C | THR | A | 9 | 42.886 | 43.939 | 52.091 | 1.00 | 32.94 | AAAA |
| ATOM | 57 | O | THR | A | 9 | 41.705 | 43.625 | 51.993 | 1.00 | 33.62 | AAAA |
| ATOM | 58 | N | LEU | A | 10 | 43.396 | 45.009 | 51.485 | 1.00 | 33.20 | AAAA |
| ATOM | 59 | CA | LEU | A | 10 | 42.573 | 45.840 | 50.611 | 1.00 | 33.29 | AAAA |
| ATOM | 60 | CB | LEU | A | 10 | 43.117 | 47.275 | 50.484 | 1.00 | 33.12 | AAAA |
| ATOM | 61 | CG | LEU | A | 10 | 43.242 | 48.245 | 51.666 | 1.00 | 32.95 | AAAA |
| ATOM | 62 | CD1 | LEU | A | 10 | 41.743 | 48.386 | 52.288 | 1.00 | 31.99 | AAAA |
| ATOM | 63 | CD2 | LEU | A | 10 | 44.126 | 47.734 | 52.675 | 1.00 | 34.71 | AAAA |
| ATOM | 64 | C | LEU | A | 10 | 42.527 | 45.231 | 49.218 | 1.00 | 33.18 | AAAA |
| ATOM | 65 | O | LEU | A | 10 | 41.876 | 45.768 | 48.328 | 1.00 | 32.52 | AAAA |
| ATOM | 66 | N | ASP | A | 11 | 43.230 | 44.121 | 49.022 | 1.00 | 33.56 | AAAA |

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Figure 19-2

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 67 | CA | ASP | A | 11 | 43.240 | 43.489 | 47.716 | 1.00 | 34.24 | AAAA |
| ATOM | 68 | CB | ASP | A | 11 | 44.393 | 42.499 | 47.607 | 1.00 | 35.81 | AAAA |
| ATOM | 69 | CG | ASP | A | 11 | 45.739 | 43.190 | 47.604 | 1.00 | 37.57 | AAAA |
| ATOM | 70 | OD1 | ASP | A | 11 | 45.890 | 44.178 | 46.855 | 1.00 | 37.95 | AAAA |
| ATOM | 71 | OD2 | ASP | A | 11 | 46.650 | 42.750 | 48.332 | 1.00 | 40.31 | AAAA |
| ATOM | 72 | C | ASP | A | 11 | 41.929 | 42.813 | 47.341 | 1.00 | 34.03 | AAAA |
| ATOM | 73 | O | ASP | A | 11 | 41.629 | 42.652 | 46.150 | 1.00 | 34.80 | AAAA |
| ATOM | 74 | N | TYR | A | 12 | 41.142 | 42.417 | 48.335 | 1.00 | 32.34 | AAAA |
| ATOM | 75 | CA | TYR | A | 12 | 39.871 | 41.803 | 48.017 | 1.00 | 32.53 | AAAA |
| ATOM | 76 | CB | TYR | A | 12 | 39.043 | 41.569 | 49.290 | 1.00 | 31.32 | AAAA |
| ATOM | 77 | CG | TYR | A | 12 | 39.551 | 40.438 | 50.162 | 1.00 | 29.95 | AAAA |
| ATOM | 78 | CD1 | TYR | A | 12 | 39.983 | 40.669 | 51.469 | 1.00 | 28.52 | AAAA |
| ATOM | 79 | CE1 | TYR | A | 12 | 40.413 | 39.614 | 52.279 | 1.00 | 28.03 | AAAA |
| ATOM | 80 | CD2 | TYR | A | 12 | 39.568 | 39.128 | 49.688 | 1.00 | 28.47 | AAAA |
| ATOM | 81 | CE2 | TYR | A | 12 | 39.992 | 38.083 | 50.483 | 1.00 | 28.47 | AAAA |
| ATOM | 82 | CZ | TYR | A | 12 | 40.408 | 38.330 | 51.775 | 1.00 | 28.43 | AAAA |
| ATOM | 83 | OH | TYR | A | 12 | 40.786 | 37.277 | 52.569 | 1.00 | 29.86 | AAAA |
| ATOM | 84 | C | TYR | A | 12 | 39.146 | 42.749 | 47.066 | 1.00 | 33.16 | AAAA |
| ATOM | 85 | O | TYR | A | 12 | 38.554 | 42.324 | 46.082 | 1.00 | 33.36 | AAAA |
| ATOM | 86 | N | GLY | A | 13 | 39.237 | 44.041 | 47.356 | 1.00 | 34.76 | AAAA |
| ATOM | 87 | CA | GLY | A | 13 | 38.594 | 45.065 | 46.546 | 1.00 | 36.60 | AAAA |
| ATOM | 88 | C | GLY | A | 13 | 38.814 | 44.961 | 45.052 | 1.00 | 37.85 | AAAA |
| ATOM | 89 | O | GLY | A | 13 | 38.105 | 45.591 | 44.275 | 1.00 | 37.40 | AAAA |
| ATOM | 90 | N | LYS | A | 14 | 39.799 | 44.171 | 44.647 | 1.00 | 39.55 | AAAA |
| ATOM | 91 | CA | LYS | A | 14 | 40.091 | 43.981 | 43.231 | 1.00 | 40.66 | AAAA |
| ATOM | 92 | CB | LYS | A | 14 | 41.605 | 43.977 | 42.995 | 1.00 | 42.26 | AAAA |
| ATOM | 93 | CG | LYS | A | 14 | 42.300 | 45.309 | 43.239 | 1.00 | 44.54 | AAAA |
| ATOM | 94 | CD | LYS | A | 14 | 41.820 | 46.445 | 42.304 | 1.00 | 46.32 | AAAA |
| ATOM | 95 | CE | LYS | A | 14 | 42.033 | 46.158 | 40.810 | 1.00 | 46.64 | AAAA |
| ATOM | 96 | NZ | LYS | A | 14 | 41.133 | 45.086 | 40.256 | 1.00 | 47.23 | AAAA |
| ATOM | 97 | C | LYS | A | 14 | 39.499 | 42.675 | 42.707 | 1.00 | 40.35 | AAAA |
| ATOM | 98 | O | LYS | A | 14 | 39.593 | 42.377 | 41.511 | 1.00 | 39.97 | AAAA |
| ATOM | 99 | N | TYR | A | 15 | 38.897 | 41.901 | 43.605 | 1.00 | 39.95 | AAAA |
| ATOM | 100 | CA | TYR | A | 15 | 38.300 | 40.617 | 43.245 | 1.00 | 40.30 | AAAA |
| ATOM | 101 | CB | TYR | A | 15 | 38.962 | 39.490 | 44.050 | 1.00 | 38.46 | AAAA |
| ATOM | 102 | CG | TYR | A | 15 | 40.472 | 39.519 | 44.021 | 1.00 | 37.01 | AAAA |
| ATOM | 103 | CD1 | TYR | A | 15 | 41.213 | 39.136 | 45.137 | 1.00 | 36.24 | AAAA |
| ATOM | 104 | CE1 | TYR | A | 15 | 42.604 | 39.220 | 45.144 | 1.00 | 35.73 | AAAA |
| ATOM | 105 | CD2 | TYR | A | 15 | 41.163 | 39.976 | 42.902 | 1.00 | 36.84 | AAAA |
| ATOM | 106 | CE2 | TYR | A | 15 | 42.556 | 40.064 | 42.898 | 1.00 | 36.53 | AAAA |
| ATOM | 107 | CZ | TYR | A | 15 | 43.271 | 39.689 | 44.028 | 1.00 | 36.24 | AAAA |
| ATOM | 108 | OH | TYR | A | 15 | 44.648 | 39.816 | 44.042 | 1.00 | 36.49 | AAAA |
| ATOM | 109 | C | TYR | A | 15 | 36.802 | 40.647 | 43.556 | 1.00 | 41.98 | AAAA |
| ATOM | 110 | O | TYR | A | 15 | 36.288 | 39.786 | 44.280 | 1.00 | 42.59 | AAAA |
| ATOM | 111 | N | ARG | A | 16 | 36.101 | 41.638 | 43.014 | 1.00 | 42.81 | AAAA |
| ATOM | 112 | CA | ARG | A | 16 | 34.670 | 41.753 | 43.257 | 1.00 | 43.47 | AAAA |
| ATOM | 113 | CB | ARG | A | 16 | 34.205 | 43.197 | 43.111 | 1.00 | 45.27 | AAAA |
| ATOM | 114 | CG | ARG | A | 16 | 35.021 | 44.234 | 43.833 | 1.00 | 48.06 | AAAA |
| ATOM | 115 | CD | ARG | A | 16 | 34.891 | 44.196 | 45.339 | 1.00 | 49.63 | AAAA |
| ATOM | 116 | NE | ARG | A | 16 | 35.632 | 45.322 | 45.905 | 1.00 | 51.65 | AAAA |
| ATOM | 117 | CZ | ARG | A | 16 | 35.382 | 46.602 | 45.622 | 1.00 | 52.71 | AAAA |
| ATOM | 118 | NH1 | ARG | A | 16 | 34.406 | 46.931 | 44.781 | 1.00 | 53.28 | AAAA |
| ATOM | 119 | NH2 | ARG | A | 16 | 36.124 | 47.560 | 46.162 | 1.00 | 53.43 | AAAA |
| ATOM | 120 | C | ARG | A | 16 | 33.913 | 40.929 | 42.230 | 1.00 | 42.86 | AAAA |
| ATOM | 121 | O | ARG | A | 16 | 34.455 | 40.541 | 41.193 | 1.00 | 41.83 | AAAA |
| ATOM | 122 | N | TYR | A | 17 | 32.651 | 40.668 | 42.523 | 1.00 | 42.42 | AAAA |
| ATOM | 123 | CA | TYR | A | 17 | 31.818 | 39.942 | 41.590 | 1.00 | 42.76 | AAAA |
| ATOM | 124 | CB | TYR | A | 17 | 30.675 | 39.254 | 42.333 | 1.00 | 40.11 | AAAA |
| ATOM | 125 | CG | TYR | A | 17 | 31.097 | 38.061 | 43.180 | 1.00 | 38.35 | AAAA |
| ATOM | 126 | CD1 | TYR | A | 17 | 32.169 | 38.148 | 44.071 | 1.00 | 36.15 | AAAA |
| ATOM | 127 | CE1 | TYR | A | 17 | 32.519 | 37.069 | 44.874 | 1.00 | 34.76 | AAAA |
| ATOM | 128 | CD2 | TYR | A | 17 | 30.386 | 36.855 | 43.116 | 1.00 | 36.40 | AAAA |
| ATOM | 129 | CE2 | TYR | A | 17 | 30.726 | 35.776 | 43.912 | 1.00 | 35.31 | AAAA |
| ATOM | 130 | CZ | TYR | A | 17 | 31.792 | 35.887 | 44.790 | 1.00 | 35.00 | AAAA |
| ATOM | 131 | OH | TYR | A | 17 | 32.115 | 34.814 | 45.584 | 1.00 | 33.29 | AAAA |
| ATOM | 132 | C | TYR | A | 17 | 31.296 | 41.000 | 40.613 | 1.00 | 44.43 | AAAA |

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Figure 19-3

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 133 | O | TYR | A | 17 | 31.346 | 42.194 | 40.905 | 1.00 | 44.68 | AAAA |
| ATOM | 134 | N | PRO | A | 18 | 30.799 | 40.574 | 39.440 | 1.00 | 45.95 | AAAA |
| ATOM | 135 | CD | PRO | A | 18 | 30.707 | 39.175 | 38.994 | 1.00 | 46.08 | AAAA |
| ATOM | 136 | CA | PRO | A | 18 | 30.268 | 41.465 | 38.402 | 1.00 | 47.24 | AAAA |
| ATOM | 137 | CB | PRO | A | 18 | 29.854 | 40.482 | 37.312 | 1.00 | 47.69 | AAAA |
| ATOM | 138 | CG | PRO | A | 18 | 30.876 | 39.338 | 37.511 | 1.00 | 46.79 | AAAA |
| ATOM | 139 | C | PRO | A | 18 | 29.129 | 42.390 | 38.834 | 1.00 | 48.98 | AAAA |
| ATOM | 140 | O | PRO | A | 18 | 28.298 | 42.020 | 39.660 | 1.00 | 49.11 | AAAA |
| ATOM | 141 | N | LYS | A | 19 | 29.114 | 43.593 | 38.253 | 1.00 | 50.59 | AAAA |
| ATOM | 142 | CA | LYS | A | 19 | 28.125 | 44.654 | 38.519 | 1.00 | 52.10 | AAAA |
| ATOM | 143 | CB | LYS | A | 19 | 27.876 | 45.466 | 37.246 | 1.00 | 54.41 | AAAA |
| ATOM | 144 | CG | LYS | A | 19 | 29.120 | 45.911 | 36.498 | 1.00 | 57.78 | AAAA |
| ATOM | 145 | CD | LYS | A | 19 | 28.747 | 46.508 | 35.142 | 1.00 | 59.34 | AAAA |
| ATOM | 146 | CE | LYS | A | 19 | 29.978 | 46.774 | 34.288 | 1.00 | 60.33 | AAAA |
| ATOM | 147 | NZ | LYS | A | 19 | 29.616 | 47.277 | 32.932 | 1.00 | 61.03 | AAAA |
| ATOM | 148 | C | LYS | A | 19 | 26.764 | 44.162 | 39.012 | 1.00 | 51.53 | AAAA |
| ATOM | 149 | O | LYS | A | 19 | 26.281 | 44.556 | 40.071 | 1.00 | 51.54 | AAAA |
| ATOM | 150 | N | ASN | A | 20 | 26.146 | 43.314 | 38.203 | 1.00 | 50.13 | AAAA |
| ATOM | 151 | CA | ASN | A | 20 | 24.831 | 42.750 | 38.482 | 1.00 | 48.44 | AAAA |
| ATOM | 152 | CB | ASN | A | 20 | 24.336 | 42.061 | 37.209 | 1.00 | 49.67 | AAAA |
| ATOM | 153 | CG | ASN | A | 20 | 25.389 | 41.132 | 36.613 | 1.00 | 51.61 | AAAA |
| ATOM | 154 | OD1 | ASN | A | 20 | 25.677 | 40.064 | 37.154 | 1.00 | 51.70 | AAAA |
| ATOM | 155 | ND2 | ASN | A | 20 | 25.998 | 41.562 | 35.509 | 1.00 | 53.00 | AAAA |
| ATOM | 156 | C | ASN | A | 20 | 24.789 | 41.765 | 39.649 | 1.00 | 45.57 | AAAA |
| ATOM | 157 | O | ASN | A | 20 | 23.764 | 41.127 | 39.877 | 1.00 | 44.67 | AAAA |
| ATOM | 158 | N | HIS | A | 21 | 25.883 | 41.662 | 40.398 | 1.00 | 42.71 | AAAA |
| ATOM | 159 | CA | HIS | A | 21 | 25.958 | 40.709 | 41.506 | 1.00 | 40.69 | AAAA |
| ATOM | 160 | CB | HIS | A | 21 | 27.216 | 39.857 | 41.353 | 1.00 | 40.16 | AAAA |
| ATOM | 161 | CG | HIS | A | 21 | 27.186 | 38.587 | 42.140 | 1.00 | 39.93 | AAAA |
| ATOM | 162 | CD2 | HIS | A | 21 | 27.329 | 38.353 | 43.467 | 1.00 | 39.27 | AAAA |
| ATOM | 163 | ND1 | HIS | A | 21 | 26.951 | 37.359 | 41.557 | 1.00 | 39.47 | AAAA |
| ATOM | 164 | CE1 | HIS | A | 21 | 26.948 | 36.425 | 42.493 | 1.00 | 39.36 | AAAA |
| ATOM | 165 | NE2 | HIS | A | 21 | 27.174 | 37.003 | 43.660 | 1.00 | 39.44 | AAAA |
| ATOM | 166 | C | HIS | A | 21 | 25.974 | 41.349 | 42.892 | 1.00 | 38.93 | AAAA |
| ATOM | 167 | O | HIS | A | 21 | 26.660 | 42.338 | 43.116 | 1.00 | 38.78 | AAAA |
| ATOM | 168 | N | PRO | A | 22 | 25.229 | 40.778 | 43.853 | 1.00 | 37.11 | AAAA |
| ATOM | 169 | CD | PRO | A | 22 | 24.371 | 39.579 | 43.814 | 1.00 | 36.09 | AAAA |
| ATOM | 170 | CA | PRO | A | 22 | 25.224 | 41.361 | 45.199 | 1.00 | 35.81 | AAAA |
| ATOM | 171 | CB | PRO | A | 22 | 24.473 | 40.306 | 46.012 | 1.00 | 36.04 | AAAA |
| ATOM | 172 | CG | PRO | A | 22 | 23.464 | 39.810 | 45.003 | 1.00 | 36.19 | AAAA |
| ATOM | 173 | C | PRO | A | 22 | 26.638 | 41.637 | 45.751 | 1.00 | 34.39 | AAAA |
| ATOM | 174 | O | PRO | A | 22 | 26.867 | 42.653 | 46.417 | 1.00 | 34.09 | AAAA |
| ATOM | 175 | N | LEU | A | 23 | 27.572 | 40.731 | 45.451 | 1.00 | 31.98 | AAAA |
| ATOM | 176 | CA | LEU | A | 23 | 28.954 | 40.827 | 45.900 | 1.00 | 29.65 | AAAA |
| ATOM | 177 | CB | LEU | A | 23 | 29.564 | 39.432 | 46.014 | 1.00 | 27.88 | AAAA |
| ATOM | 178 | CG | LEU | A | 23 | 28.896 | 38.528 | 47.048 | 1.00 | 27.31 | AAAA |
| ATOM | 179 | CD1 | LEU | A | 23 | 29.656 | 37.217 | 47.149 | 1.00 | 26.64 | AAAA |
| ATOM | 180 | CD2 | LEU | A | 23 | 28.879 | 39.212 | 48.399 | 1.00 | 26.75 | AAAA |
| ATOM | 181 | C | LEU | A | 23 | 29.838 | 41.709 | 45.018 | 1.00 | 29.20 | AAAA |
| ATOM | 182 | O | LEU | A | 23 | 31.057 | 41.606 | 45.028 | 1.00 | 28.38 | AAAA |
| ATOM | 183 | N | LYS | A | 24 | 29.204 | 42.582 | 44.259 | 1.00 | 29.27 | AAAA |
| ATOM | 184 | CA | LYS | A | 24 | 29.903 | 43.512 | 43.389 | 1.00 | 29.30 | AAAA |
| ATOM | 185 | CB | LYS | A | 24 | 28.881 | 44.091 | 42.405 | 1.00 | 29.75 | AAAA |
| ATOM | 186 | CG | LYS | A | 24 | 29.328 | 45.265 | 41.601 | 1.00 | 32.55 | AAAA |
| ATOM | 187 | CD | LYS | A | 24 | 28.537 | 46.526 | 41.994 | 1.00 | 34.37 | AAAA |
| ATOM | 188 | CE | LYS | A | 24 | 27.025 | 46.337 | 41.835 | 1.00 | 34.32 | AAAA |
| ATOM | 189 | NZ | LYS | A | 24 | 26.221 | 47.542 | 42.208 | 1.00 | 34.37 | AAAA |
| ATOM | 190 | C | LYS | A | 24 | 30.580 | 44.620 | 44.224 | 1.00 | 28.14 | AAAA |
| ATOM | 191 | O | LYS | A | 24 | 31.617 | 45.162 | 43.840 | 1.00 | 27.93 | AAAA |
| ATOM | 192 | N | ILE | A | 25 | 29.990 | 44.919 | 45.377 | 1.00 | 27.07 | AAAA |
| ATOM | 193 | CA | ILE | A | 25 | 30.468 | 45.945 | 46.296 | 1.00 | 25.82 | AAAA |
| ATOM | 194 | CB | ILE | A | 25 | 29.425 | 46.262 | 47.364 | 1.00 | 25.37 | AAAA |
| ATOM | 195 | CG1 | ILE | A | 25 | 28.190 | 46.846 | 46.737 | 1.00 | 25.71 | AAAA |
| ATOM | 196 | CG2 | ILE | A | 25 | 29.142 | 44.979 | 48.157 | 1.00 | 25.26 | AAAA |
| ATOM | 197 | CD1 | ILE | A | 25 | 28.318 | 45.163 | 49.413 | 1.00 | 25.17 | AAAA |
| ATOM | 198 | C | ILE | A | 25 | 31.700 | 45.550 | 47.095 | 1.00 | 25.28 | AAAA |

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Figure 19-4

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 199 | O | ILE | A | 25 | 32.037 | 44.379 | 47.183 | 1.00 | 24.48 | AAAA |
| ATOM | 200 | N | PRO | A | 26 | 32.375 | 46.547 | 47.714 | 1.00 | 24.98 | AAAA |
| ATOM | 201 | CD | PRO | A | 26 | 32.062 | 47.980 | 47.638 | 1.00 | 24.98 | AAAA |
| ATOM | 202 | CA | PRO | A | 26 | 33.570 | 46.367 | 48.543 | 1.00 | 24.44 | AAAA |
| ATOM | 203 | CB | PRO | A | 26 | 34.094 | 47.792 | 48.701 | 1.00 | 24.75 | AAAA |
| ATOM | 204 | CG | PRO | A | 26 | 33.435 | 48.546 | 47.538 | 1.00 | 25.51 | AAAA |
| ATOM | 205 | C | PRO | A | 26 | 33.021 | 45.838 | 49.862 | 1.00 | 23.42 | AAAA |
| ATOM | 206 | O | PRO | A | 26 | 31.930 | 46.233 | 50.272 | 1.00 | 22.12 | AAAA |
| ATOM | 207 | N | ARG | A | 27 | 33.754 | 44.960 | 50.532 | 1.00 | 23.06 | AAAA |
| ATOM | 208 | CA | ARG | A | 27 | 33.244 | 44.421 | 51.776 | 1.00 | 23.04 | AAAA |
| ATOM | 209 | CB | ARG | A | 27 | 32.633 | 43.043 | 51.492 | 1.00 | 22.20 | AAAA |
| ATOM | 210 | CG | ARG | A | 27 | 31.463 | 43.152 | 50.503 | 1.00 | 19.84 | AAAA |
| ATOM | 211 | CD | ARG | A | 27 | 30.762 | 41.844 | 50.160 | 1.00 | 18.64 | AAAA |
| ATOM | 212 | NE | ARG | A | 27 | 30.181 | 41.168 | 51.315 | 1.00 | 16.51 | AAAA |
| ATOM | 213 | CZ | ARG | A | 27 | 30.774 | 40.188 | 51.982 | 1.00 | 16.57 | AAAA |
| ATOM | 214 | NH1 | ARG | A | 27 | 31.969 | 39.763 | 51.605 | 1.00 | 17.50 | AAAA |
| ATOM | 215 | NH2 | ARG | A | 27 | 30.185 | 39.643 | 53.038 | 1.00 | 16.45 | AAAA |
| ATOM | 216 | C | ARG | A | 27 | 34.265 | 44.381 | 52.905 | 1.00 | 23.62 | AAAA |
| ATOM | 217 | O | ARG | A | 27 | 34.107 | 45.077 | 53.919 | 1.00 | 23.69 | AAAA |
| ATOM | 218 | N | VAL | A | 28 | 35.305 | 43.570 | 52.736 | 1.00 | 24.25 | AAAA |
| ATOM | 219 | CA | VAL | A | 28 | 36.355 | 43.466 | 53.737 | 1.00 | 23.36 | AAAA |
| ATOM | 220 | CB | VAL | A | 28 | 37.022 | 42.062 | 53.671 | 1.00 | 22.75 | AAAA |
| ATOM | 221 | CG1 | VAL | A | 28 | 38.292 | 42.031 | 54.475 | 1.00 | 22.95 | AAAA |
| ATOM | 222 | CG2 | VAL | A | 28 | 36.061 | 41.011 | 54.249 | 1.00 | 22.20 | AAAA |
| ATOM | 223 | C | VAL | A | 28 | 37.363 | 44.609 | 53.511 | 1.00 | 23.70 | AAAA |
| ATOM | 224 | O | VAL | A | 28 | 37.943 | 45.156 | 54.455 | 1.00 | 22.62 | AAAA |
| ATOM | 225 | N | SER | A | 29 | 37.538 | 44.989 | 52.253 | 1.00 | 24.27 | AAAA |
| ATOM | 226 | CA | SER | A | 29 | 38.444 | 46.082 | 51.910 | 1.00 | 26.03 | AAAA |
| ATOM | 227 | CB | SER | A | 29 | 38.632 | 46.178 | 50.381 | 1.00 | 25.95 | AAAA |
| ATOM | 228 | OG | SER | A | 29 | 37.395 | 46.417 | 49.716 | 1.00 | 27.57 | AAAA |
| ATOM | 229 | C | SER | A | 29 | 37.793 | 47.354 | 52.440 | 1.00 | 25.52 | AAAA |
| ATOM | 230 | O | SER | A | 29 | 38.463 | 48.311 | 52.828 | 1.00 | 25.49 | AAAA |
| ATOM | 231 | N | LEU | A | 30 | 36.468 | 47.342 | 52.448 | 1.00 | 26.09 | AAAA |
| ATOM | 232 | CA | LEU | A | 30 | 35.692 | 48.471 | 52.926 | 1.00 | 26.39 | AAAA |
| ATOM | 233 | CB | LEU | A | 30 | 34.262 | 48.365 | 52.393 | 1.00 | 25.89 | AAAA |
| ATOM | 234 | CG | LEU | A | 30 | 33.265 | 49.470 | 52.755 | 1.00 | 27.15 | AAAA |
| ATOM | 235 | CD1 | LEU | A | 30 | 32.486 | 49.101 | 53.999 | 1.00 | 26.34 | AAAA |
| ATOM | 236 | CD2 | LEU | A | 30 | 34.015 | 50.813 | 52.897 | 1.00 | 25.81 | AAAA |
| ATOM | 237 | C | LEU | A | 30 | 35.713 | 48.534 | 54.453 | 1.00 | 26.26 | AAAA |
| ATOM | 238 | O | LEU | A | 30 | 35.731 | 49.612 | 55.037 | 1.00 | 27.50 | AAAA |
| ATOM | 239 | N | LEU | A | 31 | 35.730 | 47.379 | 55.097 | 1.00 | 25.57 | AAAA |
| ATOM | 240 | CA | LEU | A | 31 | 35.776 | 47.343 | 56.545 | 1.00 | 26.87 | AAAA |
| ATOM | 241 | CB | LEU | A | 31 | 35.752 | 45.900 | 57.029 | 1.00 | 27.28 | AAAA |
| ATOM | 242 | CG | LEU | A | 31 | 35.135 | 45.563 | 58.383 | 1.00 | 27.87 | AAAA |
| ATOM | 243 | CD1 | LEU | A | 31 | 35.855 | 44.313 | 58.906 | 1.00 | 27.01 | AAAA |
| ATOM | 244 | CD2 | LEU | A | 31 | 35.261 | 46.706 | 59.372 | 1.00 | 26.32 | AAAA |
| ATOM | 245 | C | LEU | A | 31 | 37.087 | 48.003 | 57.012 | 1.00 | 28.08 | AAAA |
| ATOM | 246 | O | LEU | A | 31 | 37.094 | 48.854 | 57.901 | 1.00 | 27.42 | AAAA |
| ATOM | 247 | N | LEU | A | 32 | 38.197 | 47.584 | 56.409 | 1.00 | 29.52 | AAAA |
| ATOM | 248 | CA | LEU | A | 32 | 39.508 | 48.121 | 56.750 | 1.00 | 30.96 | AAAA |
| ATOM | 249 | CB | LEU | A | 32 | 40.607 | 47.394 | 55.950 | 1.00 | 31.58 | AAAA |
| ATOM | 250 | CG | LEU | A | 32 | 40.792 | 45.904 | 56.293 | 1.00 | 31.63 | AAAA |
| ATOM | 251 | CD1 | LEU | A | 32 | 41.810 | 45.246 | 55.380 | 1.00 | 31.31 | AAAA |
| ATOM | 252 | CD2 | LEU | A | 32 | 41.232 | 45.780 | 57.743 | 1.00 | 32.23 | AAAA |
| ATOM | 253 | C | LEU | A | 32 | 39.599 | 49.635 | 56.543 | 1.00 | 31.59 | AAAA |
| ATOM | 254 | O | LEU | A | 32 | 40.081 | 50.345 | 57.416 | 1.00 | 31.70 | AAAA |
| ATOM | 255 | N | ARG | A | 33 | 39.140 | 50.129 | 55.398 | 1.00 | 32.72 | AAAA |
| ATOM | 256 | CA | ARG | A | 33 | 39.178 | 51.564 | 55.141 | 1.00 | 33.91 | AAAA |
| ATOM | 257 | CB | ARG | A | 33 | 38.643 | 51.903 | 53.743 | 1.00 | 35.10 | AAAA |
| ATOM | 258 | CG | ARG | A | 33 | 39.627 | 51.609 | 52.621 | 1.00 | 37.84 | AAAA |
| ATOM | 259 | CD | ARG | A | 33 | 39.310 | 52.412 | 51.374 | 1.00 | 39.33 | AAAA |
| ATOM | 260 | NE | ARG | A | 33 | 38.255 | 51.806 | 50.580 | 1.00 | 42.51 | AAAA |
| ATOM | 261 | CZ | ARG | A | 33 | 37.662 | 52.395 | 49.541 | 1.00 | 44.22 | AAAA |
| ATOM | 262 | NH1 | ARG | A | 33 | 38.016 | 53.617 | 49.163 | 1.00 | 44.61 | AAAA |
| ATOM | 263 | NH2 | ARG | A | 33 | 36.723 | 51.752 | 48.861 | 1.00 | 45.23 | AAAA |
| ATOM | 264 | C | ARG | A | 33 | 38.352 | 52.305 | 56.168 | 1.00 | 33.48 | AAAA |

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Figure 19-5

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 265 | O | ARG | A | 33 | 38.713 | 53.390 | 56.592 | 1.00 | 33.61 | AAAA |
| ATOM | 266 | N | PHE | A | 34 | 37.247 | 51.682 | 56.562 | 1.00 | 33.78 | AAAA |
| ATOM | 267 | CA | PHE | A | 34 | 36.292 | 52.233 | 57.517 | 1.00 | 33.79 | AAAA |
| ATOM | 268 | CB | PHE | A | 34 | 35.065 | 51.310 | 57.573 | 1.00 | 33.88 | AAAA |
| ATOM | 269 | CG | PHE | A | 34 | 33.925 | 51.840 | 58.405 | 1.00 | 33.16 | AAAA |
| ATOM | 270 | CD1 | PHE | A | 34 | 33.108 | 52.856 | 57.925 | 1.00 | 32.77 | AAAA |
| ATOM | 271 | CD2 | PHE | A | 34 | 33.668 | 51.315 | 59.672 | 1.00 | 33.05 | AAAA |
| ATOM | 272 | CE1 | PHE | A | 34 | 32.044 | 53.343 | 58.695 | 1.00 | 32.86 | AAAA |
| ATOM | 273 | CE2 | PHE | A | 34 | 32.607 | 51.797 | 60.454 | 1.00 | 33.07 | AAAA |
| ATOM | 274 | CZ | PHE | A | 34 | 31.794 | 52.809 | 59.966 | 1.00 | 32.58 | AAAA |
| ATOM | 275 | C | PHE | A | 34 | 36.881 | 52.414 | 58.918 | 1.00 | 34.01 | AAAA |
| ATOM | 276 | O | PHE | A | 34 | 36.903 | 53.524 | 59.455 | 1.00 | 33.49 | AAAA |
| ATOM | 277 | N | LYS | A | 35 | 37.350 | 51.324 | 59.516 | 1.00 | 34.00 | AAAA |
| ATOM | 278 | CA | LYS | A | 35 | 37.928 | 51.401 | 60.843 | 1.00 | 33.90 | AAAA |
| ATOM | 279 | CB | LYS | A | 35 | 38.230 | 50.010 | 61.362 | 1.00 | 34.07 | AAAA |
| ATOM | 280 | CG | LYS | A | 35 | 37.000 | 49.190 | 61.662 | 1.00 | 33.94 | AAAA |
| ATOM | 281 | CD | LYS | A | 35 | 37.414 | 47.810 | 62.106 | 1.00 | 35.31 | AAAA |
| ATOM | 282 | CE | LYS | A | 35 | 38.062 | 47.072 | 60.948 | 1.00 | 35.91 | AAAA |
| ATOM | 283 | NZ | LYS | A | 35 | 39.058 | 47.928 | 60.236 | 1.00 | 36.19 | AAAA |
| ATOM | 284 | C | LYS | A | 35 | 39.185 | 52.255 | 60.881 | 1.00 | 34.19 | AAAA |
| ATOM | 285 | O | LYS | A | 35 | 39.554 | 52.775 | 61.929 | 1.00 | 34.32 | AAAA |
| ATOM | 286 | N | ASP | A | 36 | 39.853 | 52.384 | 59.745 | 1.00 | 33.99 | AAAA |
| ATOM | 287 | CA | ASP | A | 36 | 41.034 | 53.216 | 59.680 | 1.00 | 35.17 | AAAA |
| ATOM | 288 | CB | ASP | A | 36 | 41.812 | 52.943 | 58.388 | 1.00 | 37.40 | AAAA |
| ATOM | 289 | CG | ASP | A | 36 | 42.964 | 53.908 | 58.186 | 1.00 | 38.64 | AAAA |
| ATOM | 290 | OD1 | ASP | A | 36 | 43.648 | 54.218 | 59.184 | 1.00 | 40.02 | AAAA |
| ATOM | 291 | OD2 | ASP | A | 36 | 43.201 | 54.341 | 57.035 | 1.00 | 38.74 | AAAA |
| ATOM | 292 | C | ASP | A | 36 | 40.568 | 54.670 | 59.724 | 1.00 | 35.85 | AAAA |
| ATOM | 293 | O | ASP | A | 36 | 41.231 | 55.527 | 60.306 | 1.00 | 36.88 | AAAA |
| ATOM | 294 | N | ALA | A | 37 | 39.420 | 54.940 | 59.111 | 1.00 | 34.96 | AAAA |
| ATOM | 295 | CA | ALA | A | 37 | 38.851 | 56.280 | 59.108 | 1.00 | 34.47 | AAAA |
| ATOM | 296 | CB | ALA | A | 37 | 37.751 | 56.373 | 58.067 | 1.00 | 33.80 | AAAA |
| ATOM | 297 | C | ALA | A | 37 | 38.291 | 56.617 | 60.499 | 1.00 | 34.66 | AAAA |
| ATOM | 298 | Q | ALA | A | 37 | 38.268 | 57.779 | 60.899 | 1.00 | 34.55 | AAAA |
| ATOM | 299 | N | MET | A | 38 | 37.830 | 55.600 | 61.226 | 1.00 | 34.24 | AAAA |
| ATOM | 300 | CA | MET | A | 38 | 37.287 | 55.794 | 62.572 | 1.00 | 33.07 | AAAA |
| ATOM | 301 | CB | MET | A | 38 | 36.289 | 54.687 | 62.917 | 1.00 | 32.82 | AAAA |
| ATOM | 302 | CG | MET | A | 38 | 35.084 | 54.559 | 61.996 | 1.00 | 32.72 | AAAA |
| ATOM | 303 | SD | MET | A | 38 | 33.980 | 55.948 | 62.101 | 1.00 | 33.65 | AAAA |
| ATOM | 304 | CE | MET | A | 38 | 33.550 | 55.878 | 63.849 | 1.00 | 33.77 | AAAA |
| ATOM | 305 | C | MET | A | 38 | 38.430 | 55.724 | 63.583 | 1.00 | 33.12 | AAAA |
| ATOM | 306 | O | MET | A | 38 | 38.226 | 55.930 | 64.777 | 1.00 | 32.82 | AAAA |
| ATOM | 307 | N | ASN | A | 39 | 39.628 | 55.428 | 63.090 | 1.00 | 32.64 | AAAA |
| ATOM | 308 | CA | ASN | A | 39 | 40.805 | 55.266 | 63.935 | 1.00 | 32.38 | AAAA |
| ATOM | 309 | CB | ASN | A | 39 | 41.200 | 56.600 | 64.589 | 1.00 | 32.93 | AAAA |
| ATOM | 310 | CG | ASN | A | 39 | 41.393 | 57.736 | 63.571 | 1.00 | 34.40 | AAAA |
| ATOM | 311 | OD1 | ASN | A | 39 | 42.180 | 57.624 | 62.630 | 1.00 | 34.98 | AAAA |
| ATOM | 312 | ND2 | ASN | A | 39 | 40.677 | 58.838 | 63.772 | 1.00 | 33.52 | AAAA |
| ATOM | 313 | C | ASN | A | 39 | 40.483 | 54.212 | 65.009 | 1.00 | 31.69 | AAAA |
| ATOM | 314 | O | ASN | A | 39 | 40.565 | 54.490 | 66.205 | 1.00 | 31.12 | AAAA |
| ATOM | 315 | N | LEU | A | 40 | 40.095 | 53.010 | 64.570 | 1.00 | 31.76 | AAAA |
| ATOM | 316 | CA | LEU | A | 40 | 39.750 | 51.898 | 65.474 | 1.00 | 32.48 | AAAA |
| ATOM | 317 | CB | LEU | A | 40 | 38.259 | 51.559 | 65.386 | 1.00 | 32.55 | AAAA |
| ATOM | 318 | CG | LEU | A | 40 | 37.231 | 52.581 | 65.879 | 1.00 | 32.84 | AAAA |
| ATOM | 319 | CD1 | LEU | A | 40 | 35.837 | 52.089 | 65.554 | 1.00 | 33.79 | AAAA |
| ATOM | 320 | CD2 | LEU | A | 40 | 37.372 | 52.798 | 67.376 | 1.00 | 32.45 | AAAA |
| ATOM | 321 | C | LEU | A | 40 | 40.555 | 50.628 | 65.187 | 1.00 | 32.92 | AAAA |
| ATOM | 322 | O | LEU | A | 40 | 40.196 | 49.530 | 65.618 | 1.00 | 31.64 | AAAA |
| ATOM | 323 | N | ILE | A | 41 | 41.652 | 50.794 | 64.464 | 1.00 | 34.12 | AAAA |
| ATOM | 324 | CA | ILE | A | 41 | 42.508 | 49.680 | 64.116 | 1.00 | 36.07 | AAAA |
| ATOM | 325 | CB | ILE | A | 41 | 42.017 | 48.991 | 62.811 | 1.00 | 35.51 | AAAA |
| ATOM | 326 | CG2 | ILE | A | 41 | 42.070 | 49.952 | 61.636 | 1.00 | 33.37 | AAAA |
| ATOM | 327 | CG1 | ILE | A | 41 | 42.898 | 47.790 | 62.480 | 1.00 | 35.97 | AAAA |
| ATOM | 328 | CD1 | ILE | A | 41 | 42.854 | 46.701 | 63.500 | 1.00 | 37.19 | AAAA |
| ATOM | 329 | C | ILE | A | 41 | 43.921 | 50.226 | 63.916 | 1.00 | 38.85 | AAAA |
| ATOM | 330 | O | ILE | A | 41 | 44.106 | 51.346 | 63.413 | 1.00 | 38.98 | AAAA |

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Figure 19-6

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 331 | N | ASP | A | 42 | 44.914 | 49.446 | 64.329 | 1.00 | 40.61 | AAAA |
| ATOM | 332 | CA | ASP | A | 42 | 46.309 | 49.843 | 64.181 | 1.00 | 42.57 | AAAA |
| ATOM | 333 | CB | ASP | A | 42 | 46.973 | 50.021 | 65.553 | 1.00 | 42.42 | AAAA |
| ATOM | 334 | CG | ASP | A | 42 | 46.316 | 51.110 | 66.381 | 1.00 | 42.27 | AAAA |
| ATOM | 335 | OD1 | ASP | A | 42 | 46.227 | 52.250 | 65.883 | 1.00 | 41.20 | AAAA |
| ATOM | 336 | OD2 | ASP | A | 42 | 45.891 | 50.833 | 67.526 | 1.00 | 43.36 | AAAA |
| ATOM | 337 | C | ASP | A | 42 | 47.011 | 48.752 | 63.392 | 1.00 | 44.05 | AAAA |
| ATOM | 338 | O | ASP | A | 42 | 46.525 | 47.620 | 63.333 | 1.00 | 44.88 | AAAA |
| ATOM | 339 | N | GLU | A | 43 | 48.147 | 49.090 | 62.789 | 1.00 | 45.10 | AAAA |
| ATOM | 340 | CA | GLU | A | 43 | 48.905 | 48.141 | 61.980 | 1.00 | 46.11 | AAAA |
| ATOM | 341 | CB | GLU | A | 43 | 50.172 | 48.796 | 61.454 | 1.00 | 46.89 | AAAA |
| ATOM | 342 | CG | GLU | A | 43 | 49.924 | 50.057 | 60.668 | 1.00 | 49.30 | AAAA |
| ATOM | 343 | CD | GLU | A | 43 | 51.187 | 50.580 | 60.028 | 1.00 | 49.67 | AAAA |
| ATOM | 344 | OE1 | GLU | A | 43 | 51.760 | 49.839 | 59.201 | 1.00 | 50.60 | AAAA |
| ATOM | 345 | OE2 | GLU | A | 43 | 51.601 | 51.714 | 60.349 | 1.00 | 49.60 | AAAA |
| ATOM | 346 | C | GLU | A | 43 | 49.290 | 46.859 | 62.701 | 1.00 | 46.27 | AAAA |
| ATOM | 347 | O | GLU | A | 43 | 49.214 | 45.773 | 62.131 | 1.00 | 46.00 | AAAA |
| ATOM | 348 | N | LYS | A | 44 | 49.708 | 46.986 | 63.954 | 1.00 | 46.52 | AAAA |
| ATOM | 349 | CA | LYS | A | 44 | 50.135 | 45.832 | 64.730 | 1.00 | 46.31 | AAAA |
| ATOM | 350 | CB | LYS | A | 44 | 50.762 | 46.306 | 66.048 | 1.00 | 48.16 | AAAA |
| ATOM | 351 | CG | LYS | A | 44 | 51.977 | 47.215 | 65.799 | 1.00 | 51.59 | AAAA |
| ATOM | 352 | CD | LYS | A | 44 | 52.641 | 47.734 | 67.071 | 1.00 | 52.87 | AAAA |
| ATOM | 353 | CE | LYS | A | 44 | 53.851 | 48.601 | 66.727 | 1.00 | 53.34 | AAAA |
| ATOM | 354 | NZ | LYS | A | 44 | 54.615 | 49.033 | 67.936 | 1.00 | 53.45 | AAAA |
| ATOM | 355 | C | LYS | A | 44 | 49.029 | 44.828 | 64.996 | 1.00 | 44.74 | AAAA |
| ATOM | 356 | O | LYS | A | 44 | 49.296 | 43.735 | 65.480 | 1.00 | 45.35 | AAAA |
| ATOM | 357 | N | GLU | A | 45 | 47.793 | 45.190 | 64.659 | 1.00 | 42.49 | AAAA |
| ATOM | 358 | CA | GLU | A | 45 | 46.638 | 44.320 | 64.894 | 1.00 | 40.54 | AAAA |
| ATOM | 359 | CB | GLU | A | 45 | 45.493 | 45.125 | 65.517 | 1.00 | 40.55 | AAAA |
| ATOM | 360 | CG | GLU | A | 45 | 45.788 | 45.731 | 66.882 | 1.00 | 38.87 | AAAA |
| ATOM | 361 | CD | GLU | A | 45 | 44.663 | 46.618 | 67.360 | 1.00 | 37.57 | AAAA |
| ATOM | 362 | OE1 | GLU | A | 45 | 44.383 | 47.631 | 66.693 | 1.00 | 36.29 | AAAA |
| ATOM | 363 | OE2 | GLU | A | 45 | 44.056 | 46.300 | 68.399 | 1.00 | 38.44 | AAAA |
| ATOM | 364 | C | GLU | A | 45 | 46.126 | 43.648 | 63.630 | 1.00 | 39.15 | AAAA |
| ATOM | 365 | O | GLU | A | 45 | 45.301 | 42.737 | 63.681 | 1.00 | 39.29 | AAAA |
| ATOM | 366 | N | LEU | A | 46 | 46.619 | 44.115 | 62.497 | 1.00 | 37.62 | AAAA |
| ATOM | 367 | CA | LEU | A | 46 | 46.219 | 43.589 | 61.211 | 1.00 | 35.88 | AAAA |
| ATOM | 368 | CB | LEU | A | 46 | 46.125 | 44.750 | 60.229 | 1.00 | 36.09 | AAAA |
| ATOM | 369 | CG | LEU | A | 46 | 45.608 | 44.550 | 58.817 | 1.00 | 36.50 | AAAA |
| ATOM | 370 | CD1 | LEU | A | 46 | 44.182 | 44.021 | 58.843 | 1.00 | 36.66 | AAAA |
| ATOM | 371 | CD2 | LEU | A | 46 | 45.646 | 45.893 | 58.113 | 1.00 | 35.85 | AAAA |
| ATOM | 372 | C | LEU | A | 46 | 47.211 | 42.542 | 60.714 | 1.00 | 34.97 | AAAA |
| ATOM | 373 | O | LEU | A | 46 | 48.424 | 42.670 | 60.900 | 1.00 | 35.72 | AAAA |
| ATOM | 374 | N | ILE | A | 47 | 46.680 | 41.484 | 60.118 | 1.00 | 33.25 | AAAA |
| ATOM | 375 | CA | ILE | A | 47 | 47.497 | 40.411 | 59.560 | 1.00 | 30.92 | AAAA |
| ATOM | 376 | CB | ILE | A | 47 | 47.144 | 39.024 | 60.167 | 1.00 | 31.22 | AAAA |
| ATOM | 377 | CG2 | ILE | A | 47 | 48.093 | 37.976 | 59.640 | 1.00 | 28.55 | AAAA |
| ATOM | 378 | CG1 | ILE | A | 47 | 47.220 | 39.063 | 61.694 | 1.00 | 32.04 | AAAA |
| ATOM | 379 | CD1 | ILE | A | 47 | 48.596 | 39.241 | 62.242 | 1.00 | 34.13 | AAAA |
| ATOM | 380 | C | ILE | A | 47 | 47.138 | 40.381 | 58.076 | 1.00 | 29.70 | AAAA |
| ATOM | 381 | O | ILE | A | 47 | 45.956 | 40.373 | 57.714 | 1.00 | 28.42 | AAAA |
| ATOM | 382 | N | LYS | A | 48 | 48.150 | 40.380 | 57.221 | 1.00 | 28.78 | AAAA |
| ATOM | 383 | CA | LYS | A | 48 | 47.920 | 40.349 | 55.784 | 1.00 | 28.42 | AAAA |
| ATOM | 384 | CB | LYS | A | 48 | 49.203 | 40.727 | 55.055 | 1.00 | 27.53 | AAAA |
| ATOM | 385 | CG | LYS | A | 48 | 49.116 | 40.695 | 53.556 | 1.00 | 28.97 | AAAA |
| ATOM | 386 | CD | LYS | A | 48 | 50.464 | 41.104 | 52.941 | 1.00 | 29.67 | AAAA |
| ATOM | 387 | CE | LYS | A | 48 | 50.493 | 40.893 | 51.432 | 1.00 | 29.41 | AAAA |
| ATOM | 388 | NZ | LYS | A | 48 | 49.409 | 41.645 | 50.764 | 1.00 | 29.68 | AAAA |
| ATOM | 389 | C | LYS | A | 48 | 47.449 | 38.950 | 55.375 | 1.00 | 27.81 | AAAA |
| ATOM | 390 | O | LYS | A | 48 | 48.024 | 37.938 | 55.787 | 1.00 | 27.96 | AAAA |
| ATOM | 391 | N | SER | A | 49 | 46.385 | 38.892 | 54.581 | 1.00 | 26.82 | AAAA |
| ATOM | 392 | CA | SER | A | 49 | 45.854 | 37.611 | 54.141 | 1.00 | 26.41 | AAAA |
| ATOM | 393 | CB | SER | A | 49 | 44.514 | 37.795 | 53.420 | 1.00 | 25.40 | AAAA |
| ATOM | 394 | OG | SER | A | 49 | 43.541 | 38.349 | 54.276 | 1.00 | 25.58 | AAAA |
| ATOM | 395 | C | SER | A | 49 | 46.814 | 36.891 | 53.207 | 1.00 | 26.03 | AAAA |
| ATOM | 396 | O | SER | A | 49 | 47.462 | 37.513 | 52.373 | 1.00 | 26.98 | AAAA |

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Figure 19-7

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 397 | N | ARG | A | 50 | 46.910 | 35.576 | 53.354 | 1.00 | 25.51 | AAAA |
| ATOM | 398 | CA | ARG | A | 50 | 47.755 | 34.794 | 52.474 | 1.00 | 25.45 | AAAA |
| ATOM | 399 | CB | ARG | A | 50 | 48.807 | 33.985 | 53.252 | 1.00 | 25.85 | AAAA |
| ATOM | 400 | CG | ARG | A | 50 | 48.229 | 32.819 | 54.009 | 1.00 | 27.16 | AAAA |
| ATOM | 401 | CD | ARG | A | 50 | 49.280 | 31.995 | 54.720 | 1.00 | 27.57 | AAAA |
| ATOM | 402 | NE | ARG | A | 50 | 48.673 | 30.896 | 55.482 | 1.00 | 27.90 | AAAA |
| ATOM | 403 | CZ | ARG | A | 50 | 48.106 | 29.820 | 54.946 | 1.00 | 28.34 | AAAA |
| ATOM | 404 | NH1 | ARG | A | 50 | 48.055 | 29.672 | 53.630 | 1.00 | 28.19 | AAAA |
| ATOM | 405 | NH2 | ARG | A | 50 | 47.592 | 28.884 | 55.735 | 1.00 | 28.62 | AAAA |
| ATOM | 406 | C | ARG | A | 50 | 46.806 | 33.834 | 51.762 | 1.00 | 24.91 | AAAA |
| ATOM | 407 | O | ARG | A | 50 | 45.740 | 33.510 | 52.283 | 1.00 | 23.57 | AAAA |
| ATOM | 408 | N | PRO | A | 51 | 47.172 | 33.392 | 50.549 | 1.00 | 24.28 | AAAA |
| ATOM | 409 | CD | PRO | A | 51 | 48.361 | 33.761 | 49.770 | 1.00 | 24.13 | AAAA |
| ATOM | 410 | CA | PRO | A | 51 | 46.355 | 32.462 | 49.776 | 1.00 | 24.18 | AAAA |
| ATOM | 411 | CB | PRO | A | 51 | 47.012 | 32.512 | 48.390 | 1.00 | 24.24 | AAAA |
| ATOM | 412 | CG | PRO | A | 51 | 47.766 | 33.862 | 48.405 | 1.00 | 24.11 | AAAA |
| ATOM | 413 | C | PRO | A | 51 | 46.473 | 31.070 | 50.393 | 1.00 | 23.69 | AAAA |
| ATOM | 414 | O | PRO | A | 51 | 47.545 | 30.680 | 50.839 | 1.00 | 24.13 | AAAA |
| ATOM | 415 | N | ALA | A | 52 | 45.381 | 30.325 | 50.422 | 1.00 | 23.36 | AAAA |
| ATOM | 416 | CA | ALA | A | 52 | 45.419 | 28.972 | 50.952 | 1.00 | 23.64 | AAAA |
| ATOM | 417 | CB | ALA | A | 52 | 44.012 | 28.405 | 51.029 | 1.00 | 23.86 | AAAA |
| ATOM | 418 | C | ALA | A | 52 | 46.260 | 28.145 | 49.994 | 1.00 | 23.58 | AAAA |
| ATOM | 419 | O | ALA | A | 52 | 46.240 | 28.383 | 48.806 | 1.00 | 24.52 | AAAA |
| ATOM | 420 | N | THR | A | 53 | 47.009 | 27.185 | 50.501 | 1.00 | 24.41 | AAAA |
| ATOM | 421 | CA | THR | A | 53 | 47.815 | 26.352 | 49.628 | 1.00 | 26.26 | AAAA |
| ATOM | 422 | CB | THR | A | 53 | 48.933 | 25.642 | 50.405 | 1.00 | 26.37 | AAAA |
| ATOM | 423 | OG1 | THR | A | 53 | 48.355 | 24.763 | 51.375 | 1.00 | 26.51 | AAAA |
| ATOM | 424 | CG2 | THR | A | 53 | 49.810 | 26.648 | 51.106 | 1.00 | 24.48 | AAAA |
| ATOM | 425 | C | THR | A | 53 | 46.889 | 25.299 | 49.034 | 1.00 | 27.63 | AAAA |
| ATOM | 426 | O | THR | A | 53 | 45.870 | 24.982 | 49.620 | 1.00 | 29.22 | AAAA |
| ATOM | 427 | N | LYS | A | 54 | 47.240 | 24.776 | 47.867 | 1.00 | 29.31 | AAAA |
| ATOM | 428 | CA | LYS | A | 54 | 46.450 | 23.752 | 47.189 | 1.00 | 30.61 | AAAA |
| ATOM | 429 | CB | LYS | A | 54 | 47.249 | 23.182 | 46.015 | 1.00 | 31.68 | AAAA |
| ATOM | 430 | CG | LYS | A | 54 | 46.585 | 22.020 | 45.304 | 1.00 | 34.38 | AAAA |
| ATOM | 431 | CD | LYS | A | 54 | 45.449 | 22.464 | 44.417 | 1.00 | 36.00 | AAAA |
| ATOM | 432 | CE | LYS | A | 54 | 45.943 | 22.850 | 43.025 | 1.00 | 37.55 | AAAA |
| ATOM | 433 | NZ | LYS | A | 54 | 46.425 | 21.664 | 42.236 | 1.00 | 37.57 | AAAA |
| ATOM | 434 | C | LYS | A | 54 | 46.127 | 22.640 | 48.170 | 1.00 | 31.26 | AAAA |
| ATOM | 435 | O | LYS | A | 54 | 45.025 | 22.097 | 48.176 | 1.00 | 31.72 | AAAA |
| ATOM | 436 | N | GLU | A | 55 | 47.102 | 22.312 | 49.006 | 1.00 | 31.88 | AAAA |
| ATOM | 437 | CA | GLU | A | 55 | 46.961 | 21.260 | 50.011 | 1.00 | 32.29 | AAAA |
| ATOM | 438 | CB | GLU | A | 55 | 48.266 | 21.089 | 50.778 | 1.00 | 34.43 | AAAA |
| ATOM | 439 | CG | GLU | A | 55 | 48.265 | 19.901 | 51.706 | 1.00 | 38.39 | AAAA |
| ATOM | 440 | CD | GLU | A | 55 | 49.513 | 19.839 | 52.584 | 1.00 | 41.46 | AAAA |
| ATOM | 441 | OE1 | GLU | A | 55 | 49.745 | 18.770 | 53.200 | 1.00 | 43.30 | AAAA |
| ATOM | 442 | OE2 | GLU | A | 55 | 50.245 | 20.859 | 52.672 | 1.00 | 42.45 | AAAA |
| ATOM | 443 | C | GLU | A | 55 | 45.851 | 21.555 | 51.013 | 1.00 | 30.43 | AAAA |
| ATOM | 444 | O | GLU | A | 55 | 45.048 | 20.681 | 51.332 | 1.00 | 30.59 | AAAA |
| ATOM | 445 | N | GLU | A | 56 | 45.822 | 22.782 | 51.517 | 1.00 | 28.23 | AAAA |
| ATOM | 446 | CA | GLU | A | 56 | 44.812 | 23.164 | 52.488 | 1.00 | 27.69 | AAAA |
| ATOM | 447 | CB | GLU | A | 56 | 45.078 | 24.588 | 52.989 | 1.00 | 27.90 | AAAA |
| ATOM | 448 | CG | GLU | A | 56 | 46.434 | 24.721 | 53.670 | 1.00 | 26.64 | AAAA |
| ATOM | 449 | CD | GLU | A | 56 | 46.769 | 26.135 | 54.098 | 1.00 | 26.35 | AAAA |
| ATOM | 450 | OE1 | GLU | A | 56 | 46.615 | 27.057 | 53.265 | 1.00 | 25.12 | AAAA |
| ATOM | 451 | OE2 | GLU | A | 56 | 47.213 | 26.315 | 55.255 | 1.00 | 25.70 | AAAA |
| ATOM | 452 | C | GLU | A | 56 | 43.408 | 23.043 | 51.914 | 1.00 | 26.99 | AAAA |
| ATOM | 453 | O | GLU | A | 56 | 42.495 | 22.574 | 52.588 | 1.00 | 26.25 | AAAA |
| ATOM | 454 | N | LEU | A | 57 | 43.252 | 23.447 | 50.659 | 1.00 | 27.26 | AAAA |
| ATOM | 455 | CA | LEU | A | 57 | 41.965 | 23.389 | 49.967 | 1.00 | 27.17 | AAAA |
| ATOM | 456 | CB | LEU | A | 57 | 42.077 | 24.063 | 48.596 | 1.00 | 26.62 | AAAA |
| ATOM | 457 | CG | LEU | A | 57 | 42.491 | 25.545 | 48.656 | 1.00 | 27.64 | AAAA |
| ATOM | 458 | CD1 | LEU | A | 57 | 42.770 | 26.108 | 47.269 | 1.00 | 26.66 | AAAA |
| ATOM | 459 | CD2 | LEU | A | 57 | 41.389 | 26.341 | 49.349 | 1.00 | 26.92 | AAAA |
| ATOM | 460 | C | LEU | A | 57 | 41.552 | 21.946 | 49.796 | 1.00 | 27.26 | AAAA |
| ATOM | 461 | O | LEU | A | 57 | 40.363 | 21.612 | 49.816 | 1.00 | 27.53 | AAAA |
| ATOM | 462 | N | LEU | A | 58 | 42.547 | 21.085 | 49.641 | 1.00 | 27.42 | AAAA |

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Figure 19-8

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 463 | CA | LEU | A | 58 | 42.293 | 19.675 | 49.457 | 1.00 | 26.10 | AAAA |
| ATOM | 464 | CB | LEU | A | 58 | 43.486 | 19.019 | 48.794 | 1.00 | 25.43 | AAAA |
| ATOM | 465 | CG | LEU | A | 58 | 43.623 | 19.577 | 47.385 | 1.00 | 26.66 | AAAA |
| ATOM | 466 | CD1 | LEU | A | 58 | 44.760 | 18.884 | 46.705 | 1.00 | 27.12 | AAAA |
| ATOM | 467 | CD2 | LEU | A | 58 | 42.334 | 19.355 | 46.600 | 1.00 | 26.43 | AAAA |
| ATOM | 468 | C | LEU | A | 58 | 41.938 | 18.956 | 50.731 | 1.00 | 25.79 | AAAA |
| ATOM | 469 | O | LEU | A | 58 | 41.648 | 17.763 | 50.692 | 1.00 | 26.50 | AAAA |
| ATOM | 470 | N | LEU | A | 59 | 41.977 | 19.666 | 51.858 | 1.00 | 24.91 | AAAA |
| ATOM | 471 | CA | LEU | A | 59 | 41.595 | 19.070 | 53.136 | 1.00 | 25.15 | AAAA |
| ATOM | 472 | CB | LEU | A | 59 | 41.958 | 19.991 | 54.322 | 1.00 | 25.44 | AAAA |
| ATOM | 473 | CG | LEU | A | 59 | 43.423 | 20.280 | 54.710 | 1.00 | 24.67 | AAAA |
| ATOM | 474 | CD1 | LEU | A | 59 | 43.502 | 21.461 | 55.652 | 1.00 | 23.70 | AAAA |
| ATOM | 475 | CD2 | LEU | A | 59 | 44.044 | 19.044 | 55.357 | 1.00 | 24.08 | AAAA |
| ATOM | 476 | C | LEU | A | 59 | 40.074 | 18.870 | 53.090 | 1.00 | 25.41 | AAAA |
| ATOM | 477 | O | LEU | A | 59 | 39.503 | 18.266 | 53.993 | 1.00 | 25.88 | AAAA |
| ATOM | 478 | N | PHE | A | 60 | 39.436 | 19.392 | 52.031 | 1.00 | 25.05 | AAAA |
| ATOM | 479 | CA | PHE | A | 60 | 37.983 | 19.276 | 51.823 | 1.00 | 24.11 | AAAA |
| ATOM | 480 | CB | PHE | A | 60 | 37.250 | 20.476 | 52.440 | 1.00 | 21.80 | AAAA |
| ATOM | 481 | CG | PHE | A | 60 | 35.778 | 20.534 | 52.098 | 1.00 | 20.07 | AAAA |
| ATOM | 482 | CD1 | PHE | A | 60 | 34.917 | 19.501 | 52.462 | 1.00 | 19.27 | AAAA |
| ATOM | 483 | CD2 | PHE | A | 60 | 35.249 | 21.628 | 51.399 | 1.00 | 19.82 | AAAA |
| ATOM | 484 | CE1 | PHE | A | 60 | 33.550 | 19.557 | 52.136 | 1.00 | 19.26 | AAAA |
| ATOM | 485 | CE2 | PHE | A | 60 | 33.890 | 21.688 | 51.071 | 1.00 | 17.45 | AAAA |
| ATOM | 486 | CZ | PHE | A | 60 | 33.042 | 20.652 | 51.440 | 1.00 | 17.92 | AAAA |
| ATOM | 487 | C | PHE | A | 60 | 37.557 | 19.139 | 50.345 | 1.00 | 24.02 | AAAA |
| ATOM | 488 | O | PHE | A | 60 | 36.846 | 18.201 | 49.974 | 1.00 | 23.27 | AAAA |
| ATOM | 489 | N | HIS | A | 61 | 37.982 | 20.079 | 49.511 | 1.00 | 24.40 | AAAA |
| ATOM | 490 | CA | HIS | A | 61 | 37.626 | 20.053 | 48.099 | 1.00 | 25.04 | AAAA |
| ATOM | 491 | CB | HIS | A | 61 | 37.768 | 21.449 | 47.494 | 1.00 | 24.19 | AAAA |
| ATOM | 492 | CG | HIS | A | 61 | 36.744 | 22.429 | 47.979 | 1.00 | 24.44 | AAAA |
| ATOM | 493 | CD2 | HIS | A | 61 | 35.429 | 22.559 | 47.683 | 1.00 | 24.12 | AAAA |
| ATOM | 494 | ND1 | HIS | A | 61 | 37.038 | 23.444 | 48.864 | 1.00 | 24.36 | AAAA |
| ATOM | 495 | CE1 | HIS | A | 61 | 35.952 | 24.159 | 49.089 | 1.00 | 23.18 | AAAA |
| ATOM | 496 | NE2 | HIS | A | 61 | 34.962 | 23.643 | 48.385 | 1.00 | 23.91 | AAAA |
| ATOM | 497 | C | HIS | A | 61 | 38.416 | 19.054 | 47.253 | 1.00 | 25.60 | AAAA |
| ATOM | 498 | O | HIS | A | 61 | 39.596 | 18.805 | 47.498 | 1.00 | 26.94 | AAAA |
| ATOM | 499 | N | THR | A | 62 | 37.754 | 18.496 | 46.244 | 1.00 | 26.68 | AAAA |
| ATOM | 500 | CA | THR | A | 62 | 38.369 | 17.522 | 45.333 | 1.00 | 28.17 | AAAA |
| ATOM | 501 | CB | THR | A | 62 | 37.290 | 16.695 | 44.614 | 1.00 | 28.15 | AAAA |
| ATOM | 502 | OG1 | THR | A | 62 | 36.544 | 17.541 | 43.731 | 1.00 | 28.10 | AAAA |
| ATOM | 503 | CG2 | THR | A | 62 | 36.334 | 16.094 | 45.629 | 1.00 | 28.24 | AAAA |
| ATOM | 504 | C | THR | A | 62 | 39.226 | 18.217 | 44.278 | 1.00 | 29.28 | AAAA |
| ATOM | 505 | O | THR | A | 62 | 38.876 | 19.286 | 43.792 | 1.00 | 29.52 | AAAA |
| ATOM | 506 | N | GLU | A | 63 | 40.344 | 17.606 | 43.912 | 1.00 | 31.33 | AAAA |
| ATOM | 507 | CA | GLU | A | 63 | 41.249 | 18.202 | 42.928 | 1.00 | 32.42 | AAAA |
| ATOM | 508 | CB | GLU | A | 63 | 42.333 | 17.219 | 42.536 | 1.00 | 34.37 | AAAA |
| ATOM | 509 | CG | GLU | A | 63 | 43.304 | 16.869 | 43.609 | 1.00 | 37.20 | AAAA |
| ATOM | 510 | CD | GLU | A | 63 | 44.427 | 16.022 | 43.052 | 1.00 | 38.79 | AAAA |
| ATOM | 511 | OE1 | GLU | A | 63 | 45.100 | 16.499 | 42.097 | 1.00 | 37.96 | AAAA |
| ATOM | 512 | OE2 | GLU | A | 63 | 44.619 | 14.892 | 43.564 | 1.00 | 39.68 | AAAA |
| ATOM | 513 | C | GLU | A | 63 | 40.607 | 18.687 | 41.639 | 1.00 | 31.96 | AAAA |
| ATOM | 514 | O | GLU | A | 63 | 40.824 | 19.816 | 41.215 | 1.00 | 32.10 | AAAA |
| ATOM | 515 | N | ASP | A | 64 | 39.845 | 17.814 | 40.998 | 1.00 | 31.52 | AAAA |
| ATOM | 516 | CA | ASP | A | 64 | 39.204 | 18.165 | 39.753 | 1.00 | 31.36 | AAAA |
| ATOM | 517 | CB | ASP | A | 64 | 38.301 | 17.018 | 39.295 | 1.00 | 33.99 | AAAA |
| ATOM | 518 | CG | ASP | A | 64 | 37.213 | 16.694 | 40.302 | 1.00 | 37.38 | AAAA |
| ATOM | 519 | OD1 | ASP | A | 64 | 36.375 | 15.801 | 40.027 | 1.00 | 39.80 | AAAA |
| ATOM | 520 | OD2 | ASP | A | 64 | 37.188 | 17.332 | 41.374 | 1.00 | 38.67 | AAAA |
| ATOM | 521 | C | ASP | A | 64 | 38.412 | 19.465 | 39.902 | 1.00 | 30.02 | AAAA |
| ATOM | 522 | O | ASP | A | 64 | 38.462 | 20.331 | 39.026 | 1.00 | 30.47 | AAAA |
| ATOM | 523 | N | TYR | A | 65 | 37.695 | 19.608 | 41.012 | 1.00 | 27.51 | AAAA |
| ATOM | 524 | CA | TYR | A | 65 | 36.918 | 20.814 | 41.248 | 1.00 | 26.03 | AAAA |
| ATOM | 525 | CB | TYR | A | 65 | 36.010 | 20.654 | 42.467 | 1.00 | 25.42 | AAAA |
| ATOM | 526 | CG | TYR | A | 65 | 35.339 | 21.946 | 42.866 | 1.00 | 24.90 | AAAA |
| ATOM | 527 | CD1 | TYR | A | 65 | 34.525 | 22.636 | 41.964 | 1.00 | 25.04 | AAAA |
| ATOM | 528 | CE1 | TYR | A | 65 | 33.914 | 23.823 | 42.308 | 1.00 | 25.01 | AAAA |

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Figure 19-9

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 529 | CD2 | TYR | A | 65 | 35.525 | 22.486 | 44.136 | 1.00 | 24.65 | AAAA |
| ATOM | 530 | CE2 | TYR | A | 65 | 34.920 | 23.677 | 44.497 | 1.00 | 25.86 | AAAA |
| ATOM | 531 | CZ | TYR | A | 65 | 34.110 | 24.349 | 43.576 | 1.00 | 26.69 | AAAA |
| ATOM | 532 | OH | TYR | A | 65 | 33.499 | 25.543 | 43.924 | 1.00 | 27.20 | AAAA |
| ATOM | 533 | C | TYR | A | 65 | 37.814 | 22.022 | 41.464 | 1.00 | 24.91 | AAAA |
| ATOM | 534 | O | TYR | A | 65 | 37.460 | 23.129 | 41.096 | 1.00 | 25.62 | AAAA |
| ATOM | 535 | N | ILE | A | 66 | 38.965 | 21.812 | 42.080 | 1.00 | 23.20 | AAAA |
| ATOM | 536 | CA | ILE | A | 66 | 39.877 | 22.902 | 42.328 | 1.00 | 22.33 | AAAA |
| ATOM | 537 | CB | ILE | A | 66 | 40.924 | 22.520 | 43.402 | 1.00 | 21.45 | AAAA |
| ATOM | 538 | CG2 | ILE | A | 66 | 41.927 | 23.652 | 43.617 | 1.00 | 20.00 | AAAA |
| ATOM | 539 | CG1 | ILE | A | 66 | 40.220 | 22.289 | 44.729 | 1.00 | 20.16 | AAAA |
| ATOM | 540 | CD1 | ILE | A | 66 | 39.528 | 23.523 | 45.228 | 1.00 | 19.68 | AAAA |
| ATOM | 541 | C | ILE | A | 66 | 40.558 | 23.261 | 41.023 | 1.00 | 22.68 | AAAA |
| ATOM | 542 | O | ILE | A | 66 | 40.636 | 24.425 | 40.665 | 1.00 | 23.19 | AAAA |
| ATOM | 543 | N | ASN | A | 67 | 41.036 | 22.262 | 40.295 | 1.00 | 22.96 | AAAA |
| ATOM | 544 | CA | ASN | A | 67 | 41.698 | 22.545 | 39.029 | 1.00 | 23.92 | AAAA |
| ATOM | 545 | CB | ASN | A | 67 | 42.292 | 21.261 | 38.395 | 1.00 | 24.24 | AAAA |
| ATOM | 546 | CG | ASN | A | 67 | 43.344 | 20.588 | 39.289 | 1.00 | 23.38 | AAAA |
| ATOM | 547 | OD1 | ASN | A | 67 | 44.196 | 21.256 | 39.859 | 1.00 | 23.47 | AAAA |
| ATOM | 548 | ND2 | ASN | A | 67 | 43.290 | 19.258 | 39.392 | 1.00 | 23.20 | AAAA |
| ATOM | 549 | C | ASN | A | 67 | 40.717 | 23.216 | 38.063 | 1.00 | 23.82 | AAAA |
| ATOM | 550 | O | ASN | A | 67 | 41.123 | 23.996 | 37.204 | 1.00 | 24.63 | AAAA |
| ATOM | 551 | N | THR | A | 68 | 39.427 | 22.928 | 38.213 | 1.00 | 24.08 | AAAA |
| ATOM | 552 | CA | THR | A | 68 | 38.428 | 23.534 | 37.343 | 1.00 | 25.28 | AAAA |
| ATOM | 553 | CB | THR | A | 68 | 37.030 | 22.904 | 37.525 | 1.00 | 24.55 | AAAA |
| ATOM | 554 | OG1 | THR | A | 68 | 37.090 | 21.500 | 37.258 | 1.00 | 24.64 | AAAA |
| ATOM | 555 | CG2 | THR | A | 68 | 36.049 | 23.534 | 36.564 | 1.00 | 23.58 | AAAA |
| ATOM | 556 | C | THR | A | 68 | 38.322 | 25.023 | 37.664 | 1.00 | 26.31 | AAAA |
| ATOM | 557 | O | THR | A | 68 | 38.114 | 25.854 | 36.771 | 1.00 | 26.69 | AAAA |
| ATOM | 558 | N | LEU | A | 69 | 38.462 | 25.351 | 38.945 | 1.00 | 26.59 | AAAA |
| ATOM | 559 | CA | LEU | A | 69 | 38.381 | 26.729 | 39.378 | 1.00 | 27.05 | AAAA |
| ATOM | 560 | CB | LEU | A | 69 | 38.321 | 26.807 | 40.904 | 1.00 | 27.15 | AAAA |
| ATOM | 561 | CG | LEU | A | 69 | 37.003 | 26.397 | 41.551 | 1.00 | 25.68 | AAAA |
| ATOM | 562 | CD1 | LEU | A | 69 | 37.088 | 26.491 | 43.062 | 1.00 | 26.30 | AAAA |
| ATOM | 563 | CD2 | LEU | A | 69 | 35.933 | 27.316 | 41.044 | 1.00 | 26.14 | AAAA |
| ATOM | 564 | C | LEU | A | 69 | 39.570 | 27.508 | 38.867 | 1.00 | 28.44 | AAAA |
| ATOM | 565 | O | LEU | A | 69 | 39.425 | 28.619 | 38.356 | 1.00 | 28.59 | AAAA |
| ATOM | 566 | N | MET | A | 70 | 40.748 | 26.914 | 39.009 | 1.00 | 29.31 | AAAA |
| ATOM | 567 | CA | MET | A | 70 | 41.981 | 27.536 | 38.571 | 1.00 | 29.89 | AAAA |
| ATOM | 568 | CB | MET | A | 70 | 43.160 | 26.692 | 39.044 | 1.00 | 31.04 | AAAA |
| ATOM | 569 | CG | MET | A | 70 | 43.164 | 26.528 | 40.562 | 1.00 | 31.79 | AAAA |
| ATOM | 570 | SD | MET | A | 70 | 44.608 | 25.684 | 41.183 | 1.00 | 32.58 | AAAA |
| ATOM | 571 | CE | MET | A | 70 | 45.859 | 26.820 | 40.670 | 1.00 | 30.82 | AAAA |
| ATOM | 572 | C | MET | A | 70 | 42.017 | 27.723 | 37.057 | 1.00 | 30.36 | AAAA |
| ATOM | 573 | O | MET | A | 70 | 42.462 | 28.769 | 36.559 | 1.00 | 30.18 | AAAA |
| ATOM | 574 | N | GLU | A | 71 | 41.538 | 26.719 | 36.328 | 1.00 | 30.34 | AAAA |
| ATOM | 575 | CA | GLU | A | 71 | 41.519 | 26.795 | 34.874 | 1.00 | 30.73 | AAAA |
| ATOM | 576 | CB | GLU | A | 71 | 41.140 | 25.442 | 34.266 | 1.00 | 33.47 | AAAA |
| ATOM | 577 | CG | GLU | A | 71 | 41.122 | 25.430 | 32.731 | 1.00 | 37.11 | AAAA |
| ATOM | 578 | CD | GLU | A | 71 | 42.513 | 25.676 | 32.093 | 1.00 | 40.49 | AAAA |
| ATOM | 579 | OE1 | GLU | A | 71 | 42.570 | 25.798 | 30.844 | 1.00 | 41.95 | AAAA |
| ATOM | 580 | OE2 | GLU | A | 71 | 43.541 | 25.738 | 32.825 | 1.00 | 40.74 | AAAA |
| ATOM | 581 | C | GLU | A | 71 | 40.537 | 27.851 | 34.392 | 1.00 | 29.78 | AAAA |
| ATOM | 582 | O | GLU | A | 71 | 40.852 | 28.642 | 33.508 | 1.00 | 27.82 | AAAA |
| ATOM | 583 | N | ALA | A | 72 | 39.352 | 27.855 | 34.992 | 1.00 | 29.85 | AAAA |
| ATOM | 584 | CA | ALA | A | 72 | 38.296 | 28.790 | 34.635 | 1.00 | 29.88 | AAAA |
| ATOM | 585 | CB | ALA | A | 72 | 37.022 | 28.432 | 35.374 | 1.00 | 29.07 | AAAA |
| ATOM | 586 | C | ALA | A | 72 | 38.667 | 30.238 | 34.907 | 1.00 | 30.78 | AAAA |
| ATOM | 587 | O | ALA | A | 72 | 38.359 | 31.122 | 34.108 | 1.00 | 31.27 | AAAA |
| ATOM | 588 | N | GLU | A | 73 | 39.336 | 30.491 | 36.023 | 1.00 | 31.07 | AAAA |
| ATOM | 589 | CA | GLU | A | 73 | 39.710 | 31.856 | 36.346 | 1.00 | 31.65 | AAAA |
| ATOM | 590 | CB | GLU | A | 73 | 40.243 | 31.954 | 37.785 | 1.00 | 30.52 | AAAA |
| ATOM | 591 | CG | GLU | A | 73 | 40.643 | 33.370 | 38.198 | 1.00 | 28.73 | AAAA |
| ATOM | 592 | CD | GLU | A | 73 | 41.076 | 33.484 | 39.651 | 1.00 | 28.77 | AAAA |
| ATOM | 593 | OE1 | GLU | A | 73 | 40.239 | 33.260 | 40.546 | 1.00 | 28.94 | AAAA |
| ATOM | 594 | OE2 | GLU | A | 73 | 42.258 | 33.795 | 39.906 | 1.00 | 28.57 | AAAA |

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Figure 19-10

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 595 | C | GLU | A | 73 | 40.726 | 32.461 | 35.378 | 1.00 | 33.54 | AAAA |
| ATOM | 596 | O | GLU | A | 73 | 40.456 | 33.499 | 34.767 | 1.00 | 34.93 | AAAA |
| ATOM | 597 | N | ARG | A | 74 | 41.885 | 31.832 | 35.214 | 1.00 | 34.35 | AAAA |
| ATOM | 598 | CA | ARG | A | 74 | 42.890 | 32.428 | 34.334 | 1.00 | 36.04 | AAAA |
| ATOM | 599 | CB | ARG | A | 74 | 44.238 | 31.710 | 34.482 | 1.00 | 36.92 | AAAA |
| ATOM | 600 | CG | ARG | A | 74 | 44.327 | 30.313 | 33.923 | 1.00 | 36.14 | AAAA |
| ATOM | 601 | CD | ARG | A | 74 | 45.508 | 29.589 | 34.543 | 1.00 | 39.55 | AAAA |
| ATOM | 602 | NE | ARG | A | 74 | 45.893 | 28.404 | 33.785 | 1.00 | 42.02 | AAAA |
| ATOM | 603 | CZ | ARG | A | 74 | 46.632 | 28.436 | 32.675 | 1.00 | 42.69 | AAAA |
| ATOM | 604 | NH1 | ARG | A | 74 | 47.071 | 29.593 | 32.191 | 1.00 | 42.76 | AAAA |
| ATOM | 605 | NH2 | ARG | A | 74 | 46.933 | 27.309 | 32.046 | 1.00 | 42.92 | AAAA |
| ATOM | 606 | C | ARG | A | 74 | 42.476 | 32.532 | 32.864 | 1.00 | 36.56 | AAAA |
| ATOM | 607 | O | ARG | A | 74 | 42.842 | 33.493 | 32.187 | 1.00 | 37.73 | AAAA |
| ATOM | 608 | N | SER | A | 75 | 41.711 | 31.567 | 32.367 | 1.00 | 36.60 | AAAA |
| ATOM | 609 | CA | SER | A | 75 | 41.248 | 31.622 | 30.987 | 1.00 | 36.82 | AAAA |
| ATOM | 610 | CB | SER | A | 75 | 40.916 | 30.218 | 30.478 | 1.00 | 36.10 | AAAA |
| ATOM | 611 | OG | SER | A | 75 | 39.736 | 29.723 | 31.083 | 1.00 | 36.39 | AAAA |
| ATOM | 612 | C | SER | A | 75 | 39.980 | 32.476 | 31.001 | 1.00 | 36.90 | AAAA |
| ATOM | 613 | O | SER | A | 75 | 39.401 | 32.791 | 29.963 | 1.00 | 36.25 | AAAA |
| ATOM | 614 | N | GLN | A | 76 | 39.568 | 32.845 | 32.208 | 1.00 | 37.62 | AAAA |
| ATOM | 615 | CA | GLN | A | 76 | 38.368 | 33.639 | 32.427 | 1.00 | 37.92 | AAAA |
| ATOM | 616 | CB | GLN | A | 76 | 38.613 | 35.100 | 32.049 | 1.00 | 38.23 | AAAA |
| ATOM | 617 | CG | GLN | A | 76 | 37.630 | 36.048 | 32.717 | 1.00 | 40.67 | AAAA |
| ATOM | 618 | CD | GLN | A | 76 | 37.929 | 36.298 | 34.199 | 1.00 | 41.40 | AAAA |
| ATOM | 619 | OE1 | GLN | A | 76 | 38.226 | 35.379 | 34.973 | 1.00 | 40.79 | AAAA |
| ATOM | 620 | NE2 | GLN | A | 76 | 37.833 | 37.556 | 34.597 | 1.00 | 42.32 | AAAA |
| ATOM | 621 | C | GLN | A | 76 | 37.223 | 33.064 | 31.600 | 1.00 | 37.75 | AAAA |
| ATOM | 622 | O | GLN | A | 76 | 36.521 | 33.789 | 30.901 | 1.00 | 38.13 | AAAA |
| ATOM | 623 | N | SER | A | 77 | 37.045 | 31.749 | 31.685 | 1.00 | 37.52 | AAAA |
| ATOM | 624 | CA | SER | A | 77 | 35.990 | 31.061 | 30.950 | 1.00 | 37.75 | AAAA |
| ATOM | 625 | CB | SER | A | 77 | 36.537 | 30.440 | 29.664 | 1.00 | 37.90 | AAAA |
| ATOM | 626 | OG | SER | A | 77 | 36.851 | 31.441 | 28.724 | 1.00 | 40.32 | AAAA |
| ATOM | 627 | C | SER | A | 77 | 35.338 | 29.960 | 31.757 | 1.00 | 37.55 | AAAA |
| ATOM | 628 | O | SER | A | 77 | 35.790 | 29.620 | 32.846 | 1.00 | 36.81 | AAAA |
| ATOM | 629 | N | VAL | A | 78 | 34.264 | 29.412 | 31.198 | 1.00 | 37.82 | AAAA |
| ATOM | 630 | CA | VAL | A | 78 | 33.538 | 28.309 | 31.812 | 1.00 | 37.99 | AAAA |
| ATOM | 631 | CB | VAL | A | 78 | 32.027 | 28.514 | 31.715 | 1.00 | 37.19 | AAAA |
| ATOM | 632 | CG1 | VAL | A | 78 | 31.310 | 27.439 | 32.497 | 1.00 | 36.84 | AAAA |
| ATOM | 633 | CG2 | VAL | A | 78 | 31.662 | 29.906 | 32.201 | 1.00 | 37.60 | AAAA |
| ATOM | 634 | C | VAL | A | 78 | 33.918 | 27.089 | 30.976 | 1.00 | 38.28 | AAAA |
| ATOM | 635 | O | VAL | A | 78 | 33.497 | 26.959 | 29.819 | 1.00 | 39.18 | AAAA |
| ATOM | 636 | N | PRO | A | 79 | 34.734 | 26.187 | 31.537 | 1.00 | 37.69 | AAAA |
| ATOM | 637 | CD | PRO | A | 79 | 35.347 | 26.167 | 32.869 | 1.00 | 37.65 | AAAA |
| ATOM | 638 | CA | PRO | A | 79 | 35.146 | 24.998 | 30.797 | 1.00 | 37.54 | AAAA |
| ATOM | 639 | CB | PRO | A | 79 | 36.127 | 24.325 | 31.759 | 1.00 | 37.45 | AAAA |
| ATOM | 640 | CG | PRO | A | 79 | 36.655 | 25.489 | 32.557 | 1.00 | 37.65 | AAAA |
| ATOM | 641 | C | PRO | A | 79 | 33.980 | 24.089 | 30.434 | 1.00 | 37.20 | AAAA |
| ATOM | 642 | O | PRO | A | 79 | 32.958 | 24.050 | 31.120 | 1.00 | 36.43 | AAAA |
| ATOM | 643 | N | LYS | A | 80 | 34.154 | 23.363 | 29.338 | 1.00 | 37.42 | AAAA |
| ATOM | 644 | CA | LYS | A | 80 | 33.160 | 22.423 | 28.855 | 1.00 | 37.35 | AAAA |
| ATOM | 645 | CB | LYS | A | 80 | 33.757 | 21.586 | 27.725 | 1.00 | 37.99 | AAAA |
| ATOM | 646 | CG | LYS | A | 80 | 32.928 | 20.379 | 27.280 | 1.00 | 38.94 | AAAA |
| ATOM | 647 | CD | LYS | A | 80 | 31.835 | 20.710 | 26.286 | 1.00 | 39.07 | AAAA |
| ATOM | 648 | CE | LYS | A | 80 | 31.320 | 19.402 | 25.688 | 1.00 | 40.43 | AAAA |
| ATOM | 649 | NZ | LYS | A | 80 | 30.498 | 19.543 | 24.450 | 1.00 | 40.48 | AAAA |
| ATOM | 650 | C | LYS | A | 80 | 32.752 | 21.515 | 30.003 | 1.00 | 36.85 | AAAA |
| ATOM | 651 | O | LYS | A | 80 | 33.610 | 20.942 | 30.676 | 1.00 | 36.56 | AAAA |
| ATOM | 652 | N | GLY | A | 81 | 31.443 | 21.408 | 30.217 | 1.00 | 35.94 | AAAA |
| ATOM | 653 | CA | GLY | A | 81 | 30.903 | 20.570 | 31.268 | 1.00 | 35.48 | AAAA |
| ATOM | 654 | C | GLY | A | 81 | 31.110 | 21.054 | 32.693 | 1.00 | 35.23 | AAAA |
| ATOM | 655 | O | GLY | A | 81 | 30.749 | 20.355 | 33.644 | 1.00 | 35.46 | AAAA |
| ATOM | 656 | N | ALA | A | 82 | 31.677 | 22.241 | 32.867 | 1.00 | 35.17 | AAAA |
| ATOM | 657 | CA | ALA | A | 82 | 31.919 | 22.743 | 34.213 | 1.00 | 35.02 | AAAA |
| ATOM | 658 | CB | ALA | A | 82 | 33.076 | 23.743 | 34.208 | 1.00 | 35.13 | AAAA |
| ATOM | 659 | C | ALA | A | 82 | 30.674 | 23.378 | 34.797 | 1.00 | 34.39 | AAAA |
| ATOM | 660 | O | ALA | A | 82 | 30.451 | 23.332 | 36.001 | 1.00 | 33.82 | AAAA |

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Figure 19-11

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 661 | N | ARG | A | 83 | 29.858 | 23.960 | 33.932 | 1.00 | 34.77 | AAAA |
| ATOM | 662 | CA | ARG | A | 83 | 28.637 | 24.613 | 34.361 | 1.00 | 35.34 | AAAA |
| ATOM | 663 | CB | ARG | A | 83 | 27.899 | 25.180 | 33.150 | 1.00 | 36.26 | AAAA |
| ATOM | 664 | CG | ARG | A | 83 | 27.045 | 26.395 | 33.464 | 1.00 | 37.09 | AAAA |
| ATOM | 665 | CD | ARG | A | 83 | 26.209 | 26.141 | 34.686 | 1.00 | 37.48 | AAAA |
| ATOM | 666 | NE | ARG | A | 83 | 25.475 | 27.310 | 35.134 | 1.00 | 37.35 | AAAA |
| ATOM | 667 | CZ | ARG | A | 83 | 24.711 | 27.311 | 36.218 | 1.00 | 37.77 | AAAA |
| ATOM | 668 | NH1 | ARG | A | 83 | 24.606 | 26.204 | 36.940 | 1.00 | 37.29 | AAAA |
| ATOM | 669 | NH2 | ARG | A | 83 | 24.040 | 28.401 | 36.568 | 1.00 | 38.34 | AAAA |
| ATOM | 670 | C | ARG | A | 83 | 27.739 | 23.603 | 35.065 | 1.00 | 36.30 | AAAA |
| ATOM | 671 | O | ARG | A | 83 | 27.232 | 23.854 | 36.154 | 1.00 | 36.17 | AAAA |
| ATOM | 672 | N | GLU | A | 84 | 27.565 | 22.450 | 34.431 | 1.00 | 37.19 | AAAA |
| ATOM | 673 | CA | GLU | A | 84 | 26.721 | 21.382 | 34.948 | 1.00 | 37.80 | AAAA |
| ATOM | 674 | CB | GLU | A | 84 | 26.466 | 20.375 | 33.833 | 1.00 | 40.55 | AAAA |
| ATOM | 675 | CG | GLU | A | 84 | 25.643 | 19.171 | 34.232 | 1.00 | 43.12 | AAAA |
| ATOM | 676 | CD | GLU | A | 84 | 25.362 | 18.268 | 33.046 | 1.00 | 44.98 | AAAA |
| ATOM | 677 | OE1 | GLU | A | 84 | 24.573 | 17.301 | 33.195 | 1.00 | 46.36 | AAAA |
| ATOM | 678 | OE2 | GLU | A | 84 | 25.937 | 18.532 | 31.962 | 1.00 | 44.94 | AAAA |
| ATOM | 679 | C | GLU | A | 84 | 27.290 | 20.657 | 36.158 | 1.00 | 37.07 | AAAA |
| ATOM | 680 | O | GLU | A | 84 | 26.642 | 20.555 | 37.199 | 1.00 | 36.17 | AAAA |
| ATOM | 681 | N | LYS | A | 85 | 28.506 | 20.152 | 35.999 | 1.00 | 36.23 | AAAA |
| ATOM | 682 | CA | LYS | A | 85 | 29.202 | 19.412 | 37.043 | 1.00 | 35.36 | AAAA |
| ATOM | 683 | CB | LYS | A | 85 | 30.449 | 18.761 | 36.437 | 1.00 | 36.96 | AAAA |
| ATOM | 684 | CG | LYS | A | 85 | 31.394 | 18.158 | 37.465 | 1.00 | 39.04 | AAAA |
| ATOM | 685 | CD | LYS | A | 85 | 30.995 | 16.766 | 37.919 | 1.00 | 40.59 | AAAA |
| ATOM | 686 | CE | LYS | A | 85 | 31.508 | 15.719 | 36.933 | 1.00 | 41.88 | AAAA |
| ATOM | 687 | NZ | LYS | A | 85 | 32.998 | 15.817 | 36.757 | 1.00 | 42.00 | AAAA |
| ATOM | 688 | C | LYS | A | 85 | 29.620 | 20.202 | 38.289 | 1.00 | 33.86 | AAAA |
| ATOM | 689 | O | LYS | A | 85 | 29.576 | 19.679 | 39.404 | 1.00 | 33.82 | AAAA |
| ATOM | 690 | N | TYR | A | 86 | 30.014 | 21.458 | 38.097 | 1.00 | 32.06 | AAAA |
| ATOM | 691 | CA | TYR | A | 86 | 30.514 | 22.279 | 39.194 | 1.00 | 29.44 | AAAA |
| ATOM | 692 | CB | TYR | A | 86 | 31.956 | 22.683 | 38.875 | 1.00 | 29.97 | AAAA |
| ATOM | 693 | CG | TYR | A | 86 | 32.872 | 21.496 | 38.621 | 1.00 | 29.99 | AAAA |
| ATOM | 694 | CD1 | TYR | A | 86 | 33.281 | 20.666 | 39.666 | 1.00 | 29.24 | AAAA |
| ATOM | 695 | CE1 | TYR | A | 86 | 34.126 | 19.582 | 39.437 | 1.00 | 29.85 | AAAA |
| ATOM | 696 | CD2 | TYR | A | 86 | 33.329 | 21.204 | 37.329 | 1.00 | 30.16 | AAAA |
| ATOM | 697 | CE2 | TYR | A | 86 | 34.173 | 20.118 | 37.087 | 1.00 | 29.61 | AAAA |
| ATOM | 698 | CZ | TYR | A | 86 | 34.570 | 19.313 | 38.148 | 1.00 | 29.79 | AAAA |
| ATOM | 699 | OH | TYR | A | 86 | 35.414 | 18.253 | 37.923 | 1.00 | 29.48 | AAAA |
| ATOM | 700 | C | TYR | A | 86 | 29.705 | 23.509 | 39.572 | 1.00 | 27.81 | AAAA |
| ATOM | 701 | O | TYR | A | 86 | 30.052 | 24.202 | 40.524 | 1.00 | 27.56 | AAAA |
| ATOM | 702 | N | ASN | A | 87 | 28.642 | 23.784 | 38.828 | 1.00 | 26.60 | AAAA |
| ATOM | 703 | CA | ASN | A | 87 | 27.777 | 24.924 | 39.111 | 1.00 | 26.56 | AAAA |
| ATOM | 704 | CB | ASN | A | 87 | 27.172 | 24.772 | 40.508 | 1.00 | 26.39 | AAAA |
| ATOM | 705 | CG | ASN | A | 87 | 25.863 | 25.544 | 40.684 | 1.00 | 26.64 | AAAA |
| ATOM | 706 | OD1 | ASN | A | 87 | 25.335 | 25.632 | 41.790 | 1.00 | 26.84 | AAAA |
| ATOM | 707 | ND2 | ASN | A | 87 | 25.330 | 26.084 | 39.597 | 1.00 | 26.33 | AAAA |
| ATOM | 708 | C | ASN | A | 87 | 28.587 | 26.217 | 39.024 | 1.00 | 26.40 | AAAA |
| ATOM | 709 | O | ASN | A | 87 | 28.430 | 27.129 | 39.832 | 1.00 | 24.80 | AAAA |
| ATOM | 710 | N | ILE | A | 88 | 29.448 | 26.273 | 38.015 | 1.00 | 27.57 | AAAA |
| ATOM | 711 | CA | ILE | A | 88 | 30.330 | 27.409 | 37.767 | 1.00 | 27.88 | AAAA |
| ATOM | 712 | CB | ILE | A | 88 | 31.817 | 26.932 | 37.648 | 1.00 | 27.38 | AAAA |
| ATOM | 713 | CG2 | ILE | A | 88 | 32.684 | 27.994 | 36.986 | 1.00 | 26.34 | AAAA |
| ATOM | 714 | CG1 | ILE | A | 88 | 32.354 | 26.543 | 39.026 | 1.00 | 28.35 | AAAA |
| ATOM | 715 | CD1 | ILE | A | 88 | 32.356 | 27.671 | 40.042 | 1.00 | 27.78 | AAAA |
| ATOM | 716 | C | ILE | A | 88 | 29.946 | 28.110 | 36.472 | 1.00 | 29.17 | AAAA |
| ATOM | 717 | O | ILE | A | 88 | 29.530 | 27.469 | 35.515 | 1.00 | 29.75 | AAAA |
| ATOM | 718 | N | GLY | A | 89 | 30.092 | 29.429 | 36.443 | 1.00 | 29.96 | AAAA |
| ATOM | 719 | CA | GLY | A | 89 | 29.791 | 30.162 | 35.229 | 1.00 | 30.24 | AAAA |
| ATOM | 720 | C | GLY | A | 89 | 28.430 | 30.805 | 35.242 | 1.00 | 30.44 | AAAA |
| ATOM | 721 | O | GLY | A | 89 | 28.177 | 31.769 | 34.514 | 1.00 | 31.14 | AAAA |
| ATOM | 722 | N | GLY | A | 90 | 27.542 | 30.268 | 36.061 | 1.00 | 30.00 | AAAA |
| ATOM | 723 | CA | GLY | A | 90 | 26.221 | 30.841 | 36.129 | 1.00 | 30.52 | AAAA |
| ATOM | 724 | C | GLY | A | 90 | 26.283 | 32.262 | 36.661 | 1.00 | 31.09 | AAAA |
| ATOM | 725 | O | GLY | A | 90 | 27.356 | 32.795 | 36.962 | 1.00 | 30.34 | AAAA |
| ATOM | 726 | N | TYR | A | 91 | 25.112 | 32.873 | 36.768 | 1.00 | 31.09 | AAAA |

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Figure 19-12

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|------|
| ATOM | 727 | CA | TYR | A | 91 | 24.977 | 34.213 | 37.290 | 1.00 | 31.27 | AAAA |
| ATOM | 728 | CB | TYR | A | 91 | 23.515 | 34.634 | 37.195 | 1.00 | 31.82 | AAAA |
| ATOM | 729 | CG | TYR | A | 91 | 23.169 | 35.825 | 38.047 | 1.00 | 31.81 | AAAA |
| ATOM | 730 | CD1 | TYR | A | 91 | 23.536 | 37.108 | 37.670 | 1.00 | 32.44 | AAAA |
| ATOM | 731 | CE1 | TYR | A | 91 | 23.250 | 38.203 | 38.475 | 1.00 | 31.88 | AAAA |
| ATOM | 732 | CD2 | TYR | A | 91 | 22.505 | 35.663 | 39.254 | 1.00 | 32.63 | AAAA |
| ATOM | 733 | CE2 | TYR | A | 91 | 22.215 | 36.754 | 40.068 | 1.00 | 32.60 | AAAA |
| ATOM | 734 | CZ | TYR | A | 91 | 22.589 | 38.016 | 39.668 | 1.00 | 31.59 | AAAA |
| ATOM | 735 | OH | TYR | A | 91 | 22.283 | 39.094 | 40.450 | 1.00 | 31.94 | AAAA |
| ATOM | 736 | C | TYR | A | 91 | 25.384 | 34.202 | 38.753 | 1.00 | 31.56 | AAAA |
| ATOM | 737 | O | TYR | A | 91 | 26.075 | 35.105 | 39.233 | 1.00 | 31.21 | AAAA |
| ATOM | 738 | N | GLU | A | 92 | 24.925 | 33.158 | 39.438 | 1.00 | 31.51 | AAAA |
| ATOM | 739 | CA | GLU | A | 92 | 25.143 | 32.941 | 40.865 | 1.00 | 32.70 | AAAA |
| ATOM | 740 | CB | GLU | A | 92 | 24.463 | 31.626 | 41.268 | 1.00 | 33.55 | AAAA |
| ATOM | 741 | CG | GLU | A | 92 | 24.174 | 31.495 | 42.747 | 1.00 | 34.16 | AAAA |
| ATOM | 742 | CD | GLU | A | 92 | 23.311 | 30.278 | 43.087 | 1.00 | 35.31 | AAAA |
| ATOM | 743 | OE1 | GLU | A | 92 | 23.857 | 29.148 | 43.152 | 1.00 | 34.30 | AAAA |
| ATOM | 744 | OE2 | GLU | A | 92 | 22.076 | 30.466 | 43.275 | 1.00 | 35.36 | AAAA |
| ATOM | 745 | C | GLU | A | 92 | 26.619 | 32.902 | 41.248 | 1.00 | 33.02 | AAAA |
| ATOM | 746 | O | GLU | A | 92 | 27.073 | 33.623 | 42.140 | 1.00 | 32.91 | AAAA |
| ATOM | 747 | N | ASN | A | 93 | 27.358 | 32.049 | 40.550 | 1.00 | 32.84 | AAAA |
| ATOM | 748 | CA | ASN | A | 93 | 28.785 | 31.861 | 40.777 | 1.00 | 31.92 | AAAA |
| ATOM | 749 | CB | ASN | A | 93 | 29.015 | 30.437 | 41.278 | 1.00 | 31.18 | AAAA |
| ATOM | 750 | CG | ASN | A | 93 | 27.948 | 29.994 | 42.259 | 1.00 | 30.34 | AAAA |
| ATOM | 751 | OD1 | ASN | A | 93 | 27.723 | 30.642 | 43.271 | 1.00 | 31.20 | AAAA |
| ATOM | 752 | ND2 | ASN | A | 93 | 27.284 | 28.892 | 41.955 | 1.00 | 29.02 | AAAA |
| ATOM | 753 | C | ASN | A | 93 | 29.442 | 32.052 | 39.411 | 1.00 | 30.84 | AAAA |
| ATOM | 754 | O | ASN | A | 93 | 29.823 | 31.082 | 38.758 | 1.00 | 30.82 | AAAA |
| ATOM | 755 | N | PRO | A | 94 | 29.605 | 33.309 | 38.975 | 1.00 | 29.56 | AAAA |
| ATOM | 756 | CD | PRO | A | 94 | 29.312 | 34.590 | 39.626 | 1.00 | 29.03 | AAAA |
| ATOM | 757 | CA | PRO | A | 94 | 30.209 | 33.564 | 37.671 | 1.00 | 28.89 | AAAA |
| ATOM | 758 | CB | PRO | A | 94 | 29.890 | 35.045 | 37.416 | 1.00 | 28.22 | AAAA |
| ATOM | 759 | CG | PRO | A | 94 | 28.839 | 35.377 | 38.435 | 1.00 | 29.50 | AAAA |
| ATOM | 760 | C | PRO | A | 94 | 31.698 | 33.351 | 37.664 | 1.00 | 28.25 | AAAA |
| ATOM | 761 | O | PRO | A | 94 | 32.308 | 32.996 | 38.671 | 1.00 | 28.21 | AAAA |
| ATOM | 762 | N | VAL | A | 95 | 32.257 | 33.593 | 36.488 | 1.00 | 27.36 | AAAA |
| ATOM | 763 | CA | VAL | A | 95 | 33.676 | 33.530 | 36.247 | 1.00 | 26.24 | AAAA |
| ATOM | 764 | CB | VAL | A | 95 | 33.945 | 33.289 | 34.741 | 1.00 | 26.10 | AAAA |
| ATOM | 765 | CG1 | VAL | A | 95 | 35.373 | 33.717 | 34.357 | 1.00 | 25.47 | AAAA |
| ATOM | 766 | CG2 | VAL | A | 95 | 33.736 | 31.826 | 34.434 | 1.00 | 25.59 | AAAA |
| ATOM | 767 | C | VAL | A | 95 | 34.178 | 34.919 | 36.647 | 1.00 | 26.56 | AAAA |
| ATOM | 768 | O | VAL | A | 95 | 33.560 | 35.937 | 36.307 | 1.00 | 27.18 | AAAA |
| ATOM | 769 | N | SER | A | 96 | 35.280 | 34.966 | 37.382 | 1.00 | 25.23 | AAAA |
| ATOM | 770 | CA | SER | A | 96 | 35.858 | 36.237 | 37.790 | 1.00 | 24.51 | AAAA |
| ATOM | 771 | CB | SER | A | 96 | 34.935 | 36.961 | 38.774 | 1.00 | 23.22 | AAAA |
| ATOM | 772 | OG | SER | A | 96 | 34.941 | 36.297 | 40.014 | 1.00 | 19.76 | AAAA |
| ATOM | 773 | C | SER | A | 96 | 37.169 | 35.920 | 38.485 | 1.00 | 24.84 | AAAA |
| ATOM | 774 | O | SER | A | 96 | 37.590 | 34.764 | 38.530 | 1.00 | 25.97 | AAAA |
| ATOM | 775 | N | TYR | A | 97 | 37.824 | 36.933 | 39.030 | 1.00 | 24.02 | AAAA |
| ATOM | 776 | CA | TYR | A | 97 | 39.047 | 36.664 | 39.744 | 1.00 | 24.55 | AAAA |
| ATOM | 777 | CB | TYR | A | 97 | 40.071 | 37.762 | 39.504 | 1.00 | 23.94 | AAAA |
| ATOM | 778 | CG | TYR | A | 97 | 40.682 | 37.636 | 38.128 | 1.00 | 23.72 | AAAA |
| ATOM | 779 | CD1 | TYR | A | 97 | 40.177 | 38.341 | 37.039 | 1.00 | 23.11 | AAAA |
| ATOM | 780 | CE1 | TYR | A | 97 | 40.700 | 38.136 | 35.758 | 1.00 | 23.50 | AAAA |
| ATOM | 781 | CE2 | TYR | A | 97 | 41.717 | 36.735 | 37.903 | 1.00 | 22.25 | AAAA |
| ATOM | 782 | CE2 | TYR | A | 97 | 42.236 | 36.526 | 36.640 | 1.00 | 22.86 | AAAA |
| ATOM | 783 | CZ | TYR | A | 97 | 41.730 | 37.217 | 35.572 | 1.00 | 23.56 | AAAA |
| ATOM | 784 | OH | TYR | A | 97 | 42.232 | 36.941 | 34.318 | 1.00 | 24.06 | AAAA |
| ATOM | 785 | C | TYR | A | 97 | 38.800 | 36.436 | 41.228 | 1.00 | 25.08 | AAAA |
| ATOM | 786 | O | TYR | A | 97 | 39.739 | 36.266 | 42.009 | 1.00 | 26.91 | AAAA |
| ATOM | 787 | N | ALA | A | 98 | 37.522 | 36.406 | 41.589 | 1.00 | 24.73 | AAAA |
| ATOM | 788 | CA | ALA | A | 98 | 37.083 | 36.159 | 42.951 | 1.00 | 24.50 | AAAA |
| ATOM | 789 | CB | ALA | A | 98 | 35.800 | 36.925 | 43.235 | 1.00 | 24.48 | AAAA |
| ATOM | 790 | C | ALA | A | 98 | 36.824 | 34.661 | 43.088 | 1.00 | 23.95 | AAAA |
| ATOM | 791 | O | ALA | A | 98 | 36.929 | 34.100 | 44.171 | 1.00 | 24.21 | AAAA |
| ATOM | 792 | N | MET | A | 99 | 36.502 | 34.011 | 41.976 | 1.00 | 23.10 | AAAA |

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Figure 19-13

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 793 | CA | MET | A | 99 | 36.208 | 32.584 | 42.000 | 1.00 | 22.61 | AAAA |
| ATOM | 794 | CB | MET | A | 99 | 35.855 | 32.089 | 40.597 | 1.00 | 23.25 | AAAA |
| ATOM | 795 | CG | MET | A | 99 | 37.009 | 32.063 | 39.607 | 1.00 | 23.22 | AAAA |
| ATOM | 796 | SD | MET | A | 99 | 36.360 | 31.808 | 37.952 | 1.00 | 25.21 | AAAA |
| ATOM | 797 | CE | MET | A | 99 | 35.328 | 30.374 | 38.258 | 1.00 | 22.04 | AAAA |
| ATOM | 798 | C | MET | A | 99 | 37.319 | 31.720 | 42.581 | 1.00 | 21.80 | AAAA |
| ATOM | 799 | O | MET | A | 99 | 37.052 | 30.695 | 43.199 | 1.00 | 21.29 | AAAA |
| ATOM | 800 | N | PHE | A | 100 | 38.567 | 32.111 | 42.380 | 1.00 | 21.87 | AAAA |
| ATOM | 801 | CA | PHE | A | 100 | 39.650 | 31.322 | 42.936 | 1.00 | 21.11 | AAAA |
| ATOM | 802 | CB | PHE | A | 100 | 40.388 | 30.552 | 41.841 | 1.00 | 20.25 | AAAA |
| ATOM | 803 | CG | PHE | A | 100 | 41.451 | 29.648 | 42.375 | 1.00 | 20.14 | AAAA |
| ATOM | 804 | CD1 | PHE | A | 100 | 41.114 | 28.462 | 43.010 | 1.00 | 20.49 | AAAA |
| ATOM | 805 | CD2 | PHE | A | 100 | 42.785 | 30.050 | 42.373 | 1.00 | 19.82 | AAAA |
| ATOM | 806 | CE1 | PHE | A | 100 | 42.090 | 27.695 | 43.646 | 1.00 | 19.54 | AAAA |
| ATOM | 807 | CE2 | PHE | A | 100 | 43.755 | 29.300 | 43.001 | 1.00 | 19.22 | AAAA |
| ATOM | 808 | CZ | PHE | A | 100 | 43.410 | 28.122 | 43.641 | 1.00 | 19.47 | AAAA |
| ATOM | 809 | C | PHE | A | 100 | 40.649 | 32.161 | 43.743 | 1.00 | 21.37 | AAAA |
| ATOM | 810 | O | PHE | A | 100 | 40.959 | 31.822 | 44.887 | 1.00 | 21.26 | AAAA |
| ATOM | 811 | N | THR | A | 101 | 41.142 | 33.252 | 43.161 | 1.00 | 20.94 | AAAA |
| ATOM | 812 | CA | THR | A | 101 | 42.119 | 34.097 | 43.847 | 1.00 | 21.95 | AAAA |
| ATOM | 813 | CB | THR | A | 101 | 42.691 | 35.181 | 42.905 | 1.00 | 22.21 | AAAA |
| ATOM | 814 | OG1 | THR | A | 101 | 43.511 | 34.552 | 41.917 | 1.00 | 22.90 | AAAA |
| ATOM | 815 | CG2 | THR | A | 101 | 43.535 | 36.186 | 43.667 | 1.00 | 21.38 | AAAA |
| ATOM | 816 | C | THR | A | 101 | 41.584 | 34.755 | 45.117 | 1.00 | 22.60 | AAAA |
| ATOM | 817 | O | THR | A | 101 | 42.248 | 34.723 | 46.147 | 1.00 | 23.38 | AAAA |
| ATOM | 818 | N | GLY | A | 102 | 40.394 | 35.343 | 45.049 | 1.00 | 22.13 | AAAA |
| ATOM | 819 | CA | GLY | A | 102 | 39.826 | 35.972 | 46.227 | 1.00 | 22.03 | AAAA |
| ATOM | 820 | C | GLY | A | 102 | 39.340 | 34.928 | 47.221 | 1.00 | 21.36 | AAAA |
| ATOM | 821 | O | GLY | A | 102 | 39.433 | 35.104 | 48.439 | 1.00 | 20.02 | AAAA |
| ATOM | 822 | N | SER | A | 103 | 38.816 | 33.833 | 46.677 | 1.00 | 21.86 | AAAA |
| ATOM | 823 | CA | SER | A | 103 | 38.311 | 32.719 | 47.466 | 1.00 | 21.68 | AAAA |
| ATOM | 824 | CB | SER | A | 103 | 37.699 | 31.668 | 46.557 | 1.00 | 21.56 | AAAA |
| ATOM | 825 | OG | SER | A | 103 | 36.604 | 32.216 | 45.857 | 1.00 | 23.67 | AAAA |
| ATOM | 826 | C | SER | A | 103 | 39.450 | 32.098 | 48.229 | 1.00 | 22.67 | AAAA |
| ATOM | 827 | O | SER | A | 103 | 39.314 | 31.806 | 49.412 | 1.00 | 22.44 | AAAA |
| ATOM | 828 | N | SER | A | 104 | 40.578 | 31.898 | 47.545 | 1.00 | 23.37 | AAAA |
| ATOM | 829 | CA | SER | A | 104 | 41.746 | 31.305 | 48.183 | 1.00 | 23.50 | AAAA |
| ATOM | 830 | CB | SER | A | 104 | 42.862 | 31.070 | 47.172 | 1.00 | 24.80 | AAAA |
| ATOM | 831 | OG | SER | A | 104 | 42.441 | 30.169 | 46.175 | 1.00 | 28.38 | AAAA |
| ATOM | 832 | C | SER | A | 104 | 42.254 | 32.230 | 49.256 | 1.00 | 22.79 | AAAA |
| ATOM | 833 | O | SER | A | 104 | 42.707 | 31.794 | 50.307 | 1.00 | 22.66 | AAAA |
| ATOM | 834 | N | LEU | A | 105 | 42.160 | 33.518 | 48.970 | 1.00 | 22.08 | AAAA |
| ATOM | 835 | CA | LEU | A | 105 | 42.626 | 34.541 | 49.870 | 1.00 | 21.70 | AAAA |
| ATOM | 836 | CB | LEU | A | 105 | 42.524 | 35.882 | 49.159 | 1.00 | 21.89 | AAAA |
| ATOM | 837 | CG | LEU | A | 105 | 43.332 | 37.038 | 49.718 | 1.00 | 23.64 | AAAA |
| ATOM | 838 | CD1 | LEU | A | 105 | 44.830 | 36.692 | 49.639 | 1.00 | 22.01 | AAAA |
| ATOM | 839 | CD2 | LEU | A | 105 | 43.004 | 38.304 | 48.919 | 1.00 | 23.60 | AAAA |
| ATOM | 840 | C | LEU | A | 105 | 41.767 | 34.525 | 51.131 | 1.00 | 22.29 | AAAA |
| ATOM | 841 | O | LEU | A | 105 | 42.277 | 34.595 | 52.249 | 1.00 | 21.95 | AAAA |
| ATOM | 842 | N | ALA | A | 106 | 40.458 | 34.429 | 50.934 | 1.00 | 22.23 | AAAA |
| ATOM | 843 | CA | ALA | A | 106 | 39.515 | 34.394 | 52.042 | 1.00 | 22.32 | AAAA |
| ATOM | 844 | CB | ALA | A | 106 | 38.068 | 34.472 | 51.526 | 1.00 | 22.05 | AAAA |
| ATOM | 845 | C | ALA | A | 106 | 39.704 | 33.126 | 52.840 | 1.00 | 21.99 | AAAA |
| ATOM | 846 | O | ALA | A | 106 | 39.578 | 33.145 | 54.061 | 1.00 | 23.18 | AAAA |
| ATOM | 847 | N | THR | A | 107 | 40.011 | 32.032 | 52.144 | 1.00 | 21.24 | AAAA |
| ATOM | 848 | CA | THR | A | 107 | 40.209 | 30.732 | 52.779 | 1.00 | 20.60 | AAAA |
| ATOM | 849 | CB | THR | A | 107 | 40.170 | 29.571 | 51.749 | 1.00 | 19.82 | AAAA |
| ATOM | 850 | OG1 | THR | A | 107 | 38.903 | 29.553 | 51.083 | 1.00 | 18.56 | AAAA |
| ATOM | 851 | CG2 | THR | A | 107 | 40.360 | 28.242 | 52.455 | 1.00 | 18.58 | AAAA |
| ATOM | 852 | C | THR | A | 107 | 41.516 | 30.630 | 53.561 | 1.00 | 21.41 | AAAA |
| ATOM | 853 | O | THR | A | 107 | 41.537 | 30.040 | 54.646 | 1.00 | 23.16 | AAAA |
| ATOM | 854 | N | GLY | A | 108 | 42.601 | 31.176 | 53.003 | 1.00 | 20.14 | AAAA |
| ATOM | 855 | CA | GLY | A | 108 | 43.878 | 31.145 | 53.684 | 1.00 | 18.20 | AAAA |
| ATOM | 856 | C | GLY | A | 108 | 43.739 | 31.933 | 54.972 | 1.00 | 18.43 | AAAA |
| ATOM | 857 | O | GLY | A | 108 | 44.335 | 31.600 | 55.998 | 1.00 | 17.52 | AAAA |
| ATOM | 858 | N | SER | A | 109 | 42.909 | 32.969 | 54.929 | 1.00 | 18.56 | AAAA |

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Figure 19-14

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 859 | CA | SER | A | 109 | 42.683 | 33.805 | 56.098 | 1.00 | 19.67 | AAAA |
| ATOM | 860 | CB | SER | A | 109 | 41.899 | 35.058 | 55.707 | 1.00 | 20.27 | AAAA |
| ATOM | 861 | OG | SER | A | 109 | 42.618 | 35.803 | 54.746 | 1.00 | 21.80 | AAAA |
| ATOM | 862 | C | SER | A | 109 | 41.955 | 33.066 | 57.219 | 1.00 | 19.61 | AAAA |
| ATOM | 863 | O | SER | A | 109 | 42.078 | 33.426 | 58.388 | 1.00 | 18.40 | AAAA |
| ATOM | 864 | N | THR | A | 110 | 41.186 | 32.042 | 56.866 | 1.00 | 19.88 | AAAA |
| ATOM | 865 | CA | THR | A | 110 | 40.493 | 31.288 | 57.891 | 1.00 | 20.51 | AAAA |
| ATOM | 866 | CB | THR | A | 110 | 39.365 | 30.438 | 57.304 | 1.00 | 20.62 | AAAA |
| ATOM | 867 | OG1 | THR | A | 110 | 38.236 | 31.284 | 57.050 | 1.00 | 20.80 | AAAA |
| ATOM | 868 | CG2 | THR | A | 110 | 38.974 | 29.313 | 58.262 | 1.00 | 20.53 | AAAA |
| ATOM | 869 | C | THR | A | 110 | 41.504 | 30.420 | 58.601 | 1.00 | 20.36 | AAAA |
| ATOM | 870 | O | THR | A | 110 | 41.455 | 30.268 | 59.822 | 1.00 | 20.78 | AAAA |
| ATOM | 871 | N | VAL | A | 111 | 42.431 | 29.855 | 57.832 | 1.00 | 20.85 | AAAA |
| ATOM | 872 | CA | VAL | A | 111 | 43.480 | 29.053 | 58.423 | 1.00 | 21.03 | AAAA |
| ATOM | 873 | CB | VAL | A | 111 | 44.318 | 28.323 | 57.345 | 1.00 | 21.05 | AAAA |
| ATOM | 874 | CG1 | VAL | A | 111 | 45.537 | 27.644 | 57.983 | 1.00 | 19.91 | AAAA |
| ATOM | 875 | CG2 | VAL | A | 111 | 43.460 | 27.281 | 56.648 | 1.00 | 18.39 | AAAA |
| ATOM | 876 | C | VAL | A | 111 | 44.374 | 30.005 | 59.232 | 1.00 | 21.84 | AAAA |
| ATOM | 877 | O | VAL | A | 111 | 44.825 | 29.671 | 60.331 | 1.00 | 22.73 | AAAA |
| ATOM | 878 | N | GLN | A | 112 | 44.612 | 31.204 | 58.712 | 1.00 | 21.62 | AAAA |
| ATOM | 879 | CA | GLN | A | 112 | 45.449 | 32.133 | 59.452 | 1.00 | 21.89 | AAAA |
| ATOM | 880 | CB | GLN | A | 112 | 45.630 | 33.450 | 58.690 | 1.00 | 22.50 | AAAA |
| ATOM | 881 | CG | GLN | A | 112 | 46.288 | 33.283 | 57.335 | 1.00 | 23.68 | AAAA |
| ATOM | 882 | CD | GLN | A | 112 | 46.414 | 34.578 | 56.569 | 1.00 | 23.18 | AAAA |
| ATOM | 883 | OE1 | GLN | A | 112 | 47.389 | 35.310 | 56.722 | 1.00 | 23.86 | AAAA |
| ATOM | 884 | NE2 | GLN | A | 112 | 45.413 | 34.879 | 55.752 | 1.00 | 21.90 | AAAA |
| ATOM | 885 | C | GLN | A | 112 | 44.766 | 32.383 | 60.774 | 1.00 | 21.84 | AAAA |
| ATOM | 886 | O | GLN | A | 112 | 45.389 | 32.316 | 61.835 | 1.00 | 22.47 | AAAA |
| ATOM | 887 | N | ALA | A | 113 | 43.468 | 32.651 | 60.700 | 1.00 | 21.34 | AAAA |
| ATOM | 888 | CA | ALA | A | 113 | 42.682 | 32.934 | 61.884 | 1.00 | 20.84 | AAAA |
| ATOM | 889 | CB | ALA | A | 113 | 41.244 | 33.172 | 61.504 | 1.00 | 18.52 | AAAA |
| ATOM | 890 | C | ALA | A | 113 | 42.795 | 31.782 | 62.865 | 1.00 | 21.75 | AAAA |
| ATOM | 891 | O | ALA | A | 113 | 42.880 | 31.985 | 64.084 | 1.00 | 22.24 | AAAA |
| ATOM | 892 | N | ILE | A | 114 | 42.797 | 30.569 | 62.329 | 1.00 | 22.54 | AAAA |
| ATOM | 893 | CA | ILE | A | 114 | 42.891 | 29.393 | 63.160 | 1.00 | 23.16 | AAAA |
| ATOM | 894 | CB | ILE | A | 114 | 42.557 | 28.146 | 62.352 | 1.00 | 23.33 | AAAA |
| ATOM | 895 | CG2 | ILE | A | 114 | 42.939 | 26.912 | 63.106 | 1.00 | 23.80 | AAAA |
| ATOM | 896 | CG1 | ILE | A | 114 | 41.058 | 28.130 | 62.047 | 1.00 | 23.48 | AAAA |
| ATOM | 897 | CD1 | ILE | A | 114 | 40.610 | 26.951 | 61.204 | 1.00 | 22.08 | AAAA |
| ATOM | 898 | C | ILE | A | 114 | 44.268 | 29.270 | 63.792 | 1.00 | 24.33 | AAAA |
| ATOM | 899 | O | ILE | A | 114 | 44.373 | 29.013 | 64.990 | 1.00 | 25.30 | AAAA |
| ATOM | 900 | N | GLU | A | 115 | 45.319 | 29.490 | 63.002 | 1.00 | 24.96 | AAAA |
| ATOM | 901 | CA | GLU | A | 115 | 46.699 | 29.395 | 63.503 | 1.00 | 26.61 | AAAA |
| ATOM | 902 | CB | GLU | A | 115 | 47.708 | 29.753 | 62.406 | 1.00 | 24.75 | AAAA |
| ATOM | 903 | CG | GLU | A | 115 | 47.444 | 29.033 | 61.103 | 1.00 | 25.80 | AAAA |
| ATOM | 904 | CD | GLU | A | 115 | 48.471 | 29.323 | 60.030 | 1.00 | 26.07 | AAAA |
| ATOM | 905 | OE1 | GLU | A | 115 | 48.911 | 30.484 | 59.940 | 1.00 | 27.15 | AAAA |
| ATOM | 906 | OE2 | GLU | A | 115 | 48.819 | 28.402 | 59.260 | 1.00 | 25.45 | AAAA |
| ATOM | 907 | C | GLU | A | 115 | 46.877 | 30.340 | 64.680 | 1.00 | 27.89 | AAAA |
| ATOM | 908 | O | GLU | A | 115 | 47.480 | 29.975 | 65.695 | 1.00 | 28.04 | AAAA |
| ATOM | 909 | N | GLU | A | 116 | 46.337 | 31.552 | 64.531 | 1.00 | 29.15 | AAAA |
| ATOM | 910 | CA | GLU | A | 116 | 46.408 | 32.579 | 65.563 | 1.00 | 29.42 | AAAA |
| ATOM | 911 | CB | GLU | A | 116 | 45.751 | 33.871 | 65.082 | 1.00 | 28.26 | AAAA |
| ATOM | 912 | CG | GLU | A | 116 | 46.482 | 34.529 | 63.945 | 1.00 | 28.93 | AAAA |
| ATOM | 913 | CD | GLU | A | 116 | 47.902 | 34.937 | 64.318 | 1.00 | 28.32 | AAAA |
| ATOM | 914 | OE1 | GLU | A | 116 | 48.081 | 35.878 | 65.123 | 1.00 | 27.68 | AAAA |
| ATOM | 915 | OE2 | GLU | A | 116 | 48.838 | 34.297 | 63.810 | 1.00 | 27.38 | AAAA |
| ATOM | 916 | C | GLU | A | 116 | 45.737 | 32.126 | 66.845 | 1.00 | 29.77 | AAAA |
| ATOM | 917 | O | GLU | A | 116 | 46.338 | 32.196 | 67.920 | 1.00 | 30.29 | AAAA |
| ATOM | 918 | N | PHE | A | 117 | 44.492 | 31.665 | 66.727 | 1.00 | 29.64 | AAAA |
| ATOM | 919 | CA | PHE | A | 117 | 43.741 | 31.204 | 67.887 | 1.00 | 29.33 | AAAA |
| ATOM | 920 | CB | PHE | A | 117 | 42.425 | 30.552 | 67.480 | 1.00 | 28.89 | AAAA |
| ATOM | 921 | CG | PHE | A | 117 | 41.604 | 30.087 | 68.651 | 1.00 | 28.93 | AAAA |
| ATOM | 922 | CD1 | PHE | A | 117 | 41.010 | 31.010 | 69.510 | 1.00 | 28.42 | AAAA |
| ATOM | 923 | CD2 | PHE | A | 117 | 41.441 | 28.723 | 68.910 | 1.00 | 29.06 | AAAA |
| ATOM | 924 | CE1 | PHE | A | 117 | 40.261 | 30.588 | 70.610 | 1.00 | 28.68 | AAAA |

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Figure 19-15

| | | | | | | | | | | | |
|------|-----|------|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 925 | CE2. | PHE | A | 117 | 40.695 | 28.284 | 70.009 | 1.00 | 29.16 | AAAA |
| ATOM | 926 | CZ | PHE | A | 117 | 40.103 | 29.227 | 70.862 | 1.00 | 29.03 | AAAA |
| ATOM | 927 | C | PHE | A | 117 | 44.545 | 30.195 | 68.671 | 1.00 | 29.22 | AAAA |
| ATOM | 928 | O | PHE | A | 117 | 44.677 | 30.315 | 69.884 | 1.00 | 30.29 | AAAA |
| ATOM | 929 | N | LEU | A | 118 | 45.066 | 29.195 | 67.965 | 1.00 | 29.24 | AAAA |
| ATOM | 930 | CA | LEU | A | 118 | 45.864 | 28.145 | 68.576 | 1.00 | 29.50 | AAAA |
| ATOM | 931 | CB | LEU | A | 118 | 46.182 | 27.047 | 67.550 | 1.00 | 28.57 | AAAA |
| ATOM | 932 | CG | LEU | A | 118 | 44.962 | 26.296 | 66.989 | 1.00 | 28.16 | AAAA |
| ATOM | 933 | CD1 | LEU | A | 118 | 45.421 | 25.090 | 66.191 | 1.00 | 25.58 | AAAA |
| ATOM | 934 | CD2 | LEU | A | 118 | 44.053 | 25.846 | 68.128 | 1.00 | 27.64 | AAAA |
| ATOM | 935 | C | LEU | A | 118 | 47.150 | 28.649 | 69.227 | 1.00 | 30.14 | AAAA |
| ATOM | 936 | O | LEU | A | 118 | 47.727 | 27.954 | 70.056 | 1.00 | 29.94 | AAAA |
| ATOM | 937 | N | LYS | A | 119 | 47.602 | 29.845 | 68.847 | 1.00 | 31.36 | AAAA |
| ATOM | 938 | CA | LYS | A | 119 | 48.798 | 30.451 | 69.448 | 1.00 | 32.52 | AAAA |
| ATOM | 939 | CB | LYS | A | 119 | 49.396 | 31.539 | 68.559 | 1.00 | 32.38 | AAAA |
| ATOM | 940 | CG | LYS | A | 119 | 49.882 | 31.108 | 67.199 | 1.00 | 33.03 | AAAA |
| ATOM | 941 | CD | LYS | A | 119 | 50.371 | 32.321 | 66.411 | 1.00 | 32.74 | AAAA |
| ATOM | 942 | CE | LYS | A | 119 | 50.681 | 31.939 | 64.972 | 1.00 | 33.94 | AAAA |
| ATOM | 943 | NZ | LYS | A | 119 | 51.125 | 33.099 | 64.152 | 1.00 | 34.93 | AAAA |
| ATOM | 944 | C | LYS | A | 119 | 48.385 | 31.143 | 70.744 | 1.00 | 33.74 | AAAA |
| ATOM | 945 | O | LYS | A | 119 | 49.218 | 31.748 | 71.413 | 1.00 | 34.85 | AAAA |
| ATOM | 946 | N | GLY | A | 120 | 47.096 | 31.079 | 71.073 | 1.00 | 33.68 | AAAA |
| ATOM | 947 | CA | GLY | A | 120 | 46.600 | 31.736 | 72.263 | 1.00 | 33.69 | AAAA |
| ATOM | 948 | C | GLY | A | 120 | 45.987 | 33.110 | 71.988 | 1.00 | 34.11 | AAAA |
| ATOM | 949 | O | GLY | A | 120 | 45.588 | 33.802 | 72.932 | 1.00 | 33.65 | AAAA |
| ATOM | 950 | N | ASN | A | 121 | 45.904 | 33.513 | 70.717 | 1.00 | 33.58 | AAAA |
| ATOM | 951 | CA | ASN | A | 121 | 45.326 | 34.820 | 70.368 | 1.00 | 33.35 | AAAA |
| ATOM | 952 | CB | ASN | A | 121 | 46.194 | 35.537 | 69.341 | 1.00 | 33.18 | AAAA |
| ATOM | 953 | CG | ASN | A | 121 | 47.570 | 35.828 | 69.859 | 1.00 | 34.31 | AAAA |
| ATOM | 954 | OD1 | ASN | A | 121 | 48.333 | 34.921 | 70.154 | 1.00 | 35.67 | AAAA |
| ATOM | 955 | ND2 | ASN | A | 121 | 47.897 | 37.096 | 69.975 | 1.00 | 34.18 | AAAA |
| ATOM | 956 | C | ASN | A | 121 | 43.888 | 34.805 | 69.839 | 1.00 | 32.85 | AAAA |
| ATOM | 957 | O | ASN | A | 121 | 43.304 | 33.751 | 69.599 | 1.00 | 32.78 | AAAA |
| ATOM | 958 | N | VAL | A | 122 | 43.338 | 36.003 | 69.655 | 1.00 | 32.47 | AAAA |
| ATOM | 959 | CA | VAL | A | 122 | 41.980 | 36.200 | 69.148 | 1.00 | 30.89 | AAAA |
| ATOM | 960 | CB | VAL | A | 122 | 41.182 | 37.145 | 70.070 | 1.00 | 31.05 | AAAA |
| ATOM | 961 | CG1 | VAL | A | 122 | 39.831 | 37.423 | 69.489 | 1.00 | 30.95 | AAAA |
| ATOM | 962 | CG2 | VAL | A | 122 | 41.038 | 36.516 | 71.440 | 1.00 | 31.19 | AAAA |
| ATOM | 963 | C | VAL | A | 122 | 42.056 | 36.805 | 67.750 | 1.00 | 30.19 | AAAA |
| ATOM | 964 | O | VAL | A | 122 | 42.694 | 37.840 | 67.535 | 1.00 | 31.28 | AAAA |
| ATOM | 965 | N | ALA | A | 123 | 41.405 | 36.147 | 66.800 | 1.00 | 28.62 | AAAA |
| ATOM | 966 | CA | ALA | A | 123 | 41.415 | 36.589 | 65.421 | 1.00 | 26.49 | AAAA |
| ATOM | 967 | CB | ALA | A | 123 | 42.323 | 35.708 | 64.599 | 1.00 | 26.51 | AAAA |
| ATOM | 968 | C | ALA | A | 123 | 40.038 | 36.570 | 64.836 | 1.00 | 25.59 | AAAA |
| ATOM | 969 | O | ALA | A | 123 | 39.173 | 35.814 | 65.252 | 1.00 | 26.27 | AAAA |
| ATOM | 970 | N | PHE | A | 124 | 39.848 | 37.421 | 62.847 | 1.00 | 25.44 | AAAA |
| ATOM | 971 | CA | PHE | A | 124 | 38.590 | 37.534 | 61.156 | 1.00 | 23.87 | AAAA |
| ATOM | 972 | CB | PHE | A | 124 | 37.832 | 38.779 | 62.646 | 1.00 | 23.58 | AAAA |
| ATOM | 973 | CG | PHE | A | 124 | 36.591 | 39.119 | 62.841 | 1.00 | 23.71 | AAAA |
| ATOM | 974 | CD1 | PHE | A | 124 | 35.668 | 38.140 | 62.495 | 1.00 | 23.44 | AAAA |
| ATOM | 975 | CD2 | PHE | A | 124 | 36.311 | 40.449 | 62.498 | 1.00 | 23.75 | AAAA |
| ATOM | 976 | CE1 | PHE | A | 124 | 34.479 | 38.483 | 61.823 | 1.00 | 23.31 | AAAA |
| ATOM | 977 | CE2 | PHE | A | 124 | 35.131 | 40.796 | 61.833 | 1.00 | 21.71 | AAAA |
| ATOM | 978 | CZ | PHE | A | 124 | 34.217 | 39.815 | 61.497 | 1.00 | 22.35 | AAAA |
| ATOM | 979 | C | PHE | A | 124 | 38.951 | 37.673 | 61.700 | 1.00 | 23.26 | AAAA |
| ATOM | 980 | O | PHE | A | 124 | 39.720 | 38.555 | 61.323 | 1.00 | 22.29 | AAAA |
| ATOM | 981 | N | ASN | A | 125 | 38.427 | 36.759 | 60.897 | 1.00 | 23.24 | AAAA |
| ATOM | 982 | CA | ASN | A | 125 | 38.622 | 36.785 | 59.457 | 1.00 | 21.08 | AAAA |
| ATOM | 983 | CB | ASN | A | 125 | 39.181 | 35.470 | 58.951 | 1.00 | 19.90 | AAAA |
| ATOM | 984 | CG | ASN | A | 125 | 39.098 | 35.360 | 57.454 | 1.00 | 20.64 | AAAA |
| ATOM | 985 | OD1 | ASN | A | 125 | 39.389 | 36.317 | 56.748 | 1.00 | 21.63 | AAAA |
| ATOM | 986 | ND2 | ASN | A | 125 | 38.721 | 34.190 | 56.956 | 1.00 | 19.93 | AAAA |
| ATOM | 987 | C | ASN | A | 125 | 37.269 | 37.059 | 58.813 | 1.00 | 20.19 | AAAA |
| ATOM | 988 | O | ASN | A | 125 | 36.469 | 36.148 | 58.579 | 1.00 | 19.21 | AAAA |
| ATOM | 989 | N | PRO | A | 126 | 36.991 | 38.340 | 58.543 | 1.00 | 19.14 | AAAA |
| ATOM | 990 | CD | PRO | A | 126 | 37.893 | 39.460 | 58.858 | 1.00 | 19.22 | AAAA |

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Figure 19-16

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|------|
| ATOM | 991 | CA | PRO A 126 | 35.766 | 38.849 | 57.932 | 1.00 | 19.52 | AAAA |
| ATOM | 992 | CB | PRO A 126 | 36.005 | 40.359 | 57.941 | 1.00 | 18.55 | AAAA |
| ATOM | 993 | CG | PRO A 126 | 37.511 | 40.465 | 57.799 | 1.00 | 17.97 | AAAA |
| ATOM | 994 | C | PRO A 126 | 35.456 | 38.313 | 56.526 | 1.00 | 19.41 | AAAA |
| ATOM | 995 | O | PRO A 126 | 34.303 | 38.349 | 56.080 | 1.00 | 19.68 | AAAA |
| ATOM | 996 | N | ALA A 127 | 36.477 | 37.814 | 55.835 | 1.00 | 18.17 | AAAA |
| ATOM | 997 | CA | ALA A 127 | 36.283 | 37.314 | 54.481 | 1.00 | 17.66 | AAAA |
| ATOM | 998 | CB | ALA A 127 | 37.547 | 37.520 | 53.658 | 1.00 | 17.08 | AAAA |
| ATOM | 999 | C | ALA A 127 | 35.875 | 35.857 | 54.443 | 1.00 | 17.46 | AAAA |
| ATOM | 1000 | O | ALA A 127 | 35.438 | 35.359 | 53.409 | 1.00 | 18.92 | AAAA |
| ATOM | 1001 | N | GLY A 128 | 36.019 | 35.180 | 55.570 | 1.00 | 15.94 | AAAA |
| ATOM | 1002 | CA | GLY A 128 | 35.685 | 33.780 | 55.642 | 1.00 | 15.45 | AAAA |
| ATOM | 1003 | C | GLY A 128 | 34.226 | 33.593 | 55.955 | 1.00 | 16.08 | AAAA |
| ATOM | 1004 | O | GLY A 128 | 33.485 | 34.557 | 55.997 | 1.00 | 15.43 | AAAA |
| ATOM | 1005 | N | GLY A 129 | 33.821 | 32.353 | 56.198 | 1.00 | 16.77 | AAAA |
| ATOM | 1006 | CA | GLY A 129 | 32.426 | 32.082 | 56.462 | 1.00 | 17.82 | AAAA |
| ATOM | 1007 | C | GLY A 129 | 31.669 | 31.822 | 55.169 | 1.00 | 18.64 | AAAA |
| ATOM | 1008 | O | GLY A 129 | 30.469 | 32.051 | 55.108 | 1.00 | 18.48 | AAAA |
| ATOM | 1009 | N | MET A 130 | 32.380 | 31.368 | 54.137 | 1.00 | 20.45 | AAAA |
| ATOM | 1010 | CA | MET A 130 | 31.790 | 31.029 | 52.826 | 1.00 | 21.60 | AAAA |
| ATOM | 1011 | CB | MET A 130 | 32.866 | 31.117 | 51.744 | 1.00 | 22.02 | AAAA |
| ATOM | 1012 | CG | MET A 130 | 33.551 | 32.472 | 51.698 | 1.00 | 21.75 | AAAA |
| ATOM | 1013 | SD | MET A 130 | 34.971 | 32.567 | 50.599 | 1.00 | 24.75 | AAAA |
| ATOM | 1014 | CE | MET A 130 | 34.268 | 32.137 | 49.048 | 1.00 | 24.40 | AAAA |
| ATOM | 1015 | C | MET A 130 | 31.328 | 29.587 | 53.002 | 1.00 | 22.08 | AAAA |
| ATOM | 1016 | O | MET A 130 | 31.970 | 28.641 | 52.546 | 1.00 | 22.98 | AAAA |
| ATOM | 1017 | N | HIS A 131 | 30.184 | 29.452 | 53.659 | 1.00 | 22.25 | AAAA |
| ATOM | 1018 | CA | HIS A 131 | 29.618 | 28.171 | 54.062 | 1.00 | 20.49 | AAAA |
| ATOM | 1019 | CB | HIS A 131 | 28.832 | 28.421 | 55.342 | 1.00 | 20.00 | AAAA |
| ATOM | 1020 | CG | HIS A 131 | 27.679 | 29.360 | 55.161 | 1.00 | 17.93 | AAAA |
| ATOM | 1021 | CD2 | HIS A 131 | 27.091 | 29.846 | 54.043 | 1.00 | 17.88 | AAAA |
| ATOM | 1022 | ND1 | HIS A 131 | 26.952 | 29.854 | 56.219 | 1.00 | 19.33 | AAAA |
| ATOM | 1023 | CE1 | HIS A 131 | 25.968 | 30.607 | 55.758 | 1.00 | 16.99 | AAAA |
| ATOM | 1024 | NE2 | HIS A 131 | 26.031 | 30.617 | 54.441 | 1.00 | 17.43 | AAAA |
| ATOM | 1025 | C | HIS A 131 | 28.763 | 27.332 | 53.141 | 1.00 | 19.97 | AAAA |
| ATOM | 1026 | O | HIS A 131 | 28.330 | 26.262 | 53.541 | 1.00 | 19.61 | AAAA |
| ATOM | 1027 | N | HIS A 132 | 28.518 | 27.796 | 51.923 | 1.00 | 20.11 | AAAA |
| ATOM | 1028 | CA | HIS A 132 | 27.673 | 27.058 | 50.994 | 1.00 | 17.76 | AAAA |
| ATOM | 1029 | CB | HIS A 132 | 26.879 | 28.044 | 50.127 | 1.00 | 16.76 | AAAA |
| ATOM | 1030 | CG | HIS A 132 | 25.824 | 28.815 | 50.862 | 1.00 | 15.35 | AAAA |
| ATOM | 1031 | CD2 | HIS A 132 | 25.567 | 30.146 | 50.920 | 1.00 | 14.15 | AAAA |
| ATOM | 1032 | ND1 | HIS A 132 | 24.804 | 28.200 | 51.557 | 1.00 | 16.15 | AAAA |
| ATOM | 1033 | CE1 | HIS A 132 | 23.966 | 29.119 | 52.005 | 1.00 | 14.13 | AAAA |
| ATOM | 1034 | NE2 | HIS A 132 | 24.405 | 30.307 | 51.632 | 1.00 | 14.65 | AAAA |
| ATOM | 1035 | C | HIS A 132 | 28.355 | 26.051 | 50.065 | 1.00 | 17.99 | AAAA |
| ATOM | 1036 | O | HIS A 132 | 27.742 | 25.053 | 49.684 | 1.00 | 18.54 | AAAA |
| ATOM | 1037 | N | ALA A 133 | 29.604 | 26.305 | 49.690 | 1.00 | 17.82 | AAAA |
| ATOM | 1038 | CA | ALA A 133 | 30.300 | 25.441 | 48.742 | 1.00 | 18.38 | AAAA |
| ATOM | 1039 | CB | ALA A 133 | 31.684 | 25.961 | 48.507 | 1.00 | 17.53 | AAAA |
| ATOM | 1040 | C | ALA A 133 | 30.366 | 23.970 | 49.130 | 1.00 | 20.92 | AAAA |
| ATOM | 1041 | O | ALA A 133 | 30.578 | 23.633 | 50.298 | 1.00 | 21.79 | AAAA |
| ATOM | 1042 | N | PHE A 134 | 30.184 | 23.086 | 48.152 | 1.00 | 20.58 | AAAA |
| ATOM | 1043 | CA | PHE A 134 | 30.258 | 21.663 | 48.455 | 1.00 | 21.38 | AAAA |
| ATOM | 1044 | CB | PHE A 134 | 29.168 | 20.860 | 47.731 | 1.00 | 19.41 | AAAA |
| ATOM | 1045 | CG | PHE A 134 | 27.772 | 21.229 | 48.126 | 1.00 | 18.32 | AAAA |
| ATOM | 1046 | CD1 | PHE A 134 | 27.027 | 22.099 | 47.357 | 1.00 | 19.22 | AAAA |
| ATOM | 1047 | CD2 | PHE A 134 | 27.193 | 20.701 | 49.271 | 1.00 | 19.14 | AAAA |
| ATOM | 1048 | CE1 | PHE A 134 | 25.714 | 22.438 | 47.726 | 1.00 | 18.56 | AAAA |
| ATOM | 1049 | CE2 | PHE A 134 | 25.889 | 21.036 | 49.644 | 1.00 | 17.72 | AAAA |
| ATOM | 1050 | CZ | PHE A 134 | 25.158 | 21.903 | 48.866 | 1.00 | 18.01 | AAAA |
| ATOM | 1051 | C | PHE A 134 | 31.625 | 21.124 | 48.081 | 1.00 | 22.90 | AAAA |
| ATOM | 1052 | O | PHE A 134 | 32.459 | 21.833 | 47.544 | 1.00 | 23.37 | AAAA |
| ATOM | 1053 | N | LYS A 135 | 31.842 | 19.861 | 48.390 | 1.00 | 24.63 | AAAA |
| ATOM | 1054 | CA | LYS A 135 | 33.095 | 19.195 | 48.122 | 1.00 | 27.16 | AAAA |
| ATOM | 1055 | CB | LYS A 135 | 32.926 | 17.714 | 48.480 | 1.00 | 28.53 | AAAA |
| ATOM | 1056 | CG | LYS A 135 | 34.133 | 16.843 | 48.292 | 1.00 | 31.01 | AAAA |

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Figure 19-17

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1057 | CD | LYS | A | 135 | 33.879 | 15.472 | 48.910 | 1.00 | 32.75 | AAAA |
| ATOM | 1058 | CE | LYS | A | 135 | 33.961 | 15.495 | 50.457 | 1.00 | 33.96 | AAAA |
| ATOM | 1059 | NZ | LYS | A | 135 | 35.371 | 15.664 | 50.976 | 1.00 | 33.04 | AAAA |
| ATOM | 1060 | C | LYS | A | 135 | 33.577 | 19.390 | 46.673 | 1.00 | 27.37 | AAAA |
| ATOM | 1061 | O | LYS | A | 135 | 34.769 | 19.596 | 46.437 | 1.00 | 27.35 | AAAA |
| ATOM | 1062 | N | SER | A | 136 | 32.658 | 19.354 | 45.714 | 1.00 | 27.32 | AAAA |
| ATOM | 1063 | CA | SER | A | 136 | 33.028 | 19.527 | 44.313 | 1.00 | 28.31 | AAAA |
| ATOM | 1064 | CB | SER | A | 136 | 33.093 | 18.162 | 43.626 | 1.00 | 28.56 | AAAA |
| ATOM | 1065 | OG | SER | A | 136 | 33.822 | 17.242 | 44.417 | 1.00 | 29.28 | AAAA |
| ATOM | 1066 | C | SER | A | 136 | 31.993 | 20.395 | 43.599 | 1.00 | 28.91 | AAAA |
| ATOM | 1067 | O | SER | A | 136 | 31.568 | 20.080 | 42.486 | 1.00 | 28.78 | AAAA |
| ATOM | 1068 | N | ARG | A | 137 | 31.595 | 21.502 | 44.212 | 1.00 | 29.08 | AAAA |
| ATOM | 1069 | CA | ARG | A | 137 | 30.574 | 22.311 | 43.576 | 1.00 | 29.66 | AAAA |
| ATOM | 1070 | CB | ARG | A | 137 | 29.259 | 21.528 | 43.657 | 1.00 | 31.65 | AAAA |
| ATOM | 1071 | CG | ARG | A | 137 | 27.989 | 22.273 | 43.355 | 1.00 | 33.89 | AAAA |
| ATOM | 1072 | CD | ARG | A | 137 | 26.862 | 21.267 | 43.373 | 1.00 | 35.93 | AAAA |
| ATOM | 1073 | NE | ARG | A | 137 | 26.961 | 20.366 | 42.228 | 1.00 | 36.31 | AAAA |
| ATOM | 1074 | CZ | ARG | A | 137 | 26.505 | 20.660 | 41.015 | 1.00 | 35.99 | AAAA |
| ATOM | 1075 | NH1 | ARG | A | 137 | 25.915 | 21.834 | 40.798 | 1.00 | 34.63 | AAAA |
| ATOM | 1076 | NH2 | ARG | A | 137 | 26.650 | 19.786 | 40.025 | 1.00 | 35.35 | AAAA |
| ATOM | 1077 | C | ARG | A | 137 | 30.402 | 23.723 | 44.116 | 1.00 | 28.53 | AAAA |
| ATOM | 1078 | O | ARG | A | 137 | 30.418 | 23.946 | 45.324 | 1.00 | 28.51 | AAAA |
| ATOM | 1079 | N | ALA | A | 138 | 30.247 | 24.673 | 43.202 | 1.00 | 27.53 | AAAA |
| ATOM | 1080 | CA | ALA | A | 138 | 30.039 | 26.063 | 43.581 | 1.00 | 27.64 | AAAA |
| ATOM | 1081 | CB | ALA | A | 138 | 30.236 | 26.984 | 42.381 | 1.00 | 27.87 | AAAA |
| ATOM | 1082 | C | ALA | A | 138 | 28.601 | 26.130 | 44.079 | 1.00 | 27.27 | AAAA |
| ATOM | 1083 | O | ALA | A | 138 | 27.769 | 25.321 | 43.671 | 1.00 | 28.30 | AAAA |
| ATOM | 1084 | N | ASN | A | 139 | 28.292 | 27.080 | 44.951 | 1.00 | 26.16 | AAAA |
| ATOM | 1085 | CA | ASN | A | 139 | 26.945 | 27.134 | 45.480 | 1.00 | 25.39 | AAAA |
| ATOM | 1086 | CB | ASN | A | 139 | 26.673 | 25.847 | 46.282 | 1.00 | 24.58 | AAAA |
| ATOM | 1087 | CG | ASN | A | 139 | 25.343 | 25.872 | 47.017 | 1.00 | 25.37 | AAAA |
| ATOM | 1088 | OD1 | ASN | A | 139 | 24.272 | 26.017 | 46.413 | 1.00 | 24.20 | AAAA |
| ATOM | 1089 | ND2 | ASN | A | 139 | 25.408 | 25.720 | 48.338 | 1.00 | 24.91 | AAAA |
| ATOM | 1090 | C | ASN | A | 139 | 26.683 | 28.358 | 46.341 | 1.00 | 24.90 | AAAA |
| ATOM | 1091 | O | ASN | A | 139 | 27.346 | 28.570 | 47.348 | 1.00 | 24.98 | AAAA |
| ATOM | 1092 | N | GLY | A | 140 | 25.702 | 29.145 | 45.916 | 1.00 | 24.46 | AAAA |
| ATOM | 1093 | CA | GLY | A | 140 | 25.294 | 30.336 | 46.625 | 1.00 | 22.96 | AAAA |
| ATOM | 1094 | C | GLY | A | 140 | 26.383 | 31.358 | 46.755 | 1.00 | 22.24 | AAAA |
| ATOM | 1095 | O | GLY | A | 140 | 26.663 | 31.817 | 47.867 | 1.00 | 23.09 | AAAA |
| ATOM | 1096 | N | PHE | A | 141 | 26.992 | 31.711 | 45.625 | 1.00 | 20.60 | AAAA |
| ATOM | 1097 | CA | PHE | A | 141 | 28.075 | 32.700 | 45.572 | 1.00 | 19.43 | AAAA |
| ATOM | 1098 | CB | PHE | A | 141 | 27.758 | 33.920 | 46.430 | 1.00 | 19.86 | AAAA |
| ATOM | 1099 | CG | PHE | A | 141 | 26.453 | 34.577 | 46.114 | 1.00 | 21.18 | AAAA |
| ATOM | 1100 | CD1 | PHE | A | 141 | 25.974 | 35.592 | 46.934 | 1.00 | 20.49 | AAAA |
| ATOM | 1101 | CD2 | PHE | A | 141 | 25.723 | 34.218 | 44.985 | 1.00 | 21.42 | AAAA |
| ATOM | 1102 | CE1 | PHE | A | 141 | 24.800 | 36.242 | 46.638 | 1.00 | 22.45 | AAAA |
| ATOM | 1103 | CE2 | PHE | A | 141 | 24.540 | 34.859 | 44.672 | 1.00 | 21.76 | AAAA |
| ATOM | 1104 | CZ | PHE | A | 141 | 24.072 | 35.881 | 45.499 | 1.00 | 23.05 | AAAA |
| ATOM | 1105 | C | PHE | A | 141 | 29.396 | 32.132 | 46.069 | 1.00 | 18.68 | AAAA |
| ATOM | 1106 | O | PHE | A | 141 | 30.438 | 32.784 | 45.944 | 1.00 | 19.19 | AAAA |
| ATOM | 1107 | N | CYS | A | 142 | 29.367 | 30.930 | 46.635 | 1.00 | 16.93 | AAAA |
| ATOM | 1108 | CA | CYS | A | 142 | 30.594 | 30.332 | 47.150 | 1.00 | 16.80 | AAAA |
| ATOM | 1109 | CB | CYS | A | 142 | 30.323 | 29.689 | 48.509 | 1.00 | 16.51 | AAAA |
| ATOM | 1110 | SG | CYS | A | 142 | 29.524 | 30.826 | 49.617 | 1.00 | 15.01 | AAAA |
| ATOM | 1111 | C | CYS | A | 142 | 31.227 | 29.315 | 46.221 | 1.00 | 16.45 | AAAA |
| ATOM | 1112 | O | CYS | A | 142 | 30.533 | 28.565 | 45.556 | 1.00 | 15.32 | AAAA |
| ATOM | 1113 | N | TYR | A | 143 | 32.558 | 29.311 | 46.190 | 1.00 | 18.39 | AAAA |
| ATOM | 1114 | CA | TYR | A | 143 | 33.340 | 28.394 | 45.362 | 1.00 | 18.63 | AAAA |
| ATOM | 1115 | CB | TYR | A | 143 | 34.298 | 29.154 | 44.438 | 1.00 | 19.48 | AAAA |
| ATOM | 1116 | CG | TYR | A | 143 | 33.664 | 30.214 | 43.571 | 1.00 | 19.55 | AAAA |
| ATOM | 1117 | CD1 | TYR | A | 143 | 33.480 | 31.510 | 44.043 | 1.00 | 20.27 | AAAA |
| ATOM | 1118 | CE1 | TYR | A | 143 | 32.856 | 32.473 | 43.261 | 1.00 | 21.63 | AAAA |
| ATOM | 1119 | CD2 | TYR | A | 143 | 33.212 | 29.910 | 42.292 | 1.00 | 20.14 | AAAA |
| ATOM | 1120 | CE2 | TYR | A | 143 | 32.588 | 30.863 | 41.507 | 1.00 | 20.82 | AAAA |
| ATOM | 1121 | CZ | TYR | A | 143 | 32.414 | 32.135 | 41.998 | 1.00 | 20.90 | AAAA |
| ATOM | 1122 | OH | TYR | A | 143 | 31.787 | 33.071 | 41.228 | 1.00 | 23.36 | AAAA |

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Figure 19-18

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1123 | C | TYR | A | 143 | 34.162 | 27.490 | 46.283 | 1.00 | 19.06 | AAAA |
| ATOM | 1124 | O | TYR | A | 143 | 34.319 | 26.289 | 46.032 | 1.00 | 18.40 | AAAA |
| ATOM | 1125 | N | ILE | A | 144 | 34.695 | 28.087 | 47.344 | 1.00 | 19.15 | AAAA |
| ATOM | 1126 | CA | ILE | A | 144 | 35.490 | 27.350 | 48.315 | 1.00 | 19.97 | AAAA |
| ATOM | 1127 | CB | ILE | A | 144 | 36.952 | 27.861 | 48.355 | 1.00 | 19.74 | AAAA |
| ATOM | 1128 | CG2 | ILE | A | 144 | 37.757 | 27.088 | 49.410 | 1.00 | 18.03 | AAAA |
| ATOM | 1129 | CG1 | ILE | A | 144 | 37.584 | 27.671 | 46.965 | 1.00 | 20.12 | AAAA |
| ATOM | 1130 | CD1 | ILE | A | 144 | 39.053 | 28.072 | 46.846 | 1.00 | 21.05 | AAAA |
| ATOM | 1131 | C | ILE | A | 144 | 34.833 | 27.532 | 49.665 | 1.00 | 20.22 | AAAA |
| ATOM | 1132 | O | ILE | A | 144 | 34.357 | 28.626 | 49.981 | 1.00 | 19.94 | AAAA |
| ATOM | 1133 | N | ASN | A | 145 | 34.787 | 26.451 | 50.440 | 1.00 | 20.57 | AAAA |
| ATOM | 1134 | CA | ASN | A | 145 | 34.165 | 26.448 | 51.770 | 1.00 | 20.39 | AAAA |
| ATOM | 1135 | CB | ASN | A | 145 | 33.450 | 25.114 | 51.990 | 1.00 | 19.39 | AAAA |
| ATOM | 1136 | CG | ASN | A | 145 | 32.505 | 25.143 | 53.171 | 1.00 | 19.31 | AAAA |
| ATOM | 1137 | OD1 | ASN | A | 145 | 32.862 | 25.583 | 54.263 | 1.00 | 21.26 | AAAA |
| ATOM | 1138 | ND2 | ASN | A | 145 | 31.290 | 24.667 | 52.960 | 1.00 | 17.08 | AAAA |
| ATOM | 1139 | C | ASN | A | 145 | 35.236 | 26.621 | 52.856 | 1.00 | 20.17 | AAAA |
| ATOM | 1140 | O | ASN | A | 145 | 35.690 | 25.622 | 53.421 | 1.00 | 19.75 | AAAA |
| ATOM | 1141 | N | ASN | A | 146 | 35.644 | 27.862 | 53.148 | 1.00 | 20.06 | AAAA |
| ATOM | 1142 | CA | ASN | A | 146 | 36.671 | 28.075 | 54.166 | 1.00 | 20.98 | AAAA |
| ATOM | 1143 | CB | ASN | A | 146 | 37.019 | 29.573 | 54.333 | 1.00 | 21.78 | AAAA |
| ATOM | 1144 | CG | ASN | A | 146 | 35.876 | 30.411 | 54.882 | 1.00 | 22.78 | AAAA |
| ATOM | 1145 | OD1 | ASN | A | 146 | 35.651 | 30.465 | 56.091 | 1.00 | 22.83 | AAAA |
| ATOM | 1146 | ND2 | ASN | A | 146 | 35.144 | 31.078 | 53.983 | 1.00 | 23.70 | AAAA |
| ATOM | 1147 | C | ASN | A | 146 | 36.307 | 27.413 | 55.496 | 1.00 | 21.18 | AAAA |
| ATOM | 1148 | O | ASN | A | 146 | 37.169 | 26.823 | 56.139 | 1.00 | 21.48 | AAAA |
| ATOM | 1149 | N | PRO | A | 147 | 35.031 | 27.476 | 55.922 | 1.00 | 20.88 | AAAA |
| ATOM | 1150 | CD | PRO | A | 147 | 33.835 | 28.120 | 55.358 | 1.00 | 21.85 | AAAA |
| ATOM | 1151 | CA | PRO | A | 147 | 34.674 | 26.831 | 57.183 | 1.00 | 21.42 | AAAA |
| ATOM | 1152 | CB | PRO | A | 147 | 33.176 | 27.073 | 57.261 | 1.00 | 21.00 | AAAA |
| ATOM | 1153 | CG | PRO | A | 147 | 33.052 | 28.408 | 56.605 | 1.00 | 20.47 | AAAA |
| ATOM | 1154 | C | PRO | A | 147 | 35.015 | 25.334 | 57.174 | 1.00 | 22.79 | AAAA |
| ATOM | 1155 | O | PRO | A | 147 | 35.650 | 24.833 | 58.099 | 1.00 | 25.69 | AAAA |
| ATOM | 1156 | N | ALA | A | 148 | 34.603 | 24.616 | 56.136 | 1.00 | 22.34 | AAAA |
| ATOM | 1157 | CA | ALA | A | 148 | 34.889 | 23.193 | 56.070 | 1.00 | 22.23 | AAAA |
| ATOM | 1158 | CB | ALA | A | 148 | 34.260 | 22.561 | 54.825 | 1.00 | 22.87 | AAAA |
| ATOM | 1159 | C | ALA | A | 148 | 36.378 | 22.998 | 56.054 | 1.00 | 22.33 | AAAA |
| ATOM | 1160 | O | ALA | A | 148 | 36.912 | 22.249 | 56.861 | 1.00 | 23.42 | AAAA |
| ATOM | 1161 | N | VAL | A | 149 | 37.050 | 23.661 | 55.122 | 1.00 | 22.50 | AAAA |
| ATOM | 1162 | CA | VAL | A | 149 | 38.505 | 23.569 | 55.018 | 1.00 | 21.29 | AAAA |
| ATOM | 1163 | CB | VAL | A | 149 | 39.066 | 24.581 | 54.002 | 1.00 | 20.46 | AAAA |
| ATOM | 1164 | CG1 | VAL | A | 149 | 40.578 | 24.607 | 54.085 | 1.00 | 19.36 | AAAA |
| ATOM | 1165 | CG2 | VAL | A | 149 | 38.608 | 24.229 | 52.593 | 1.00 | 20.03 | AAAA |
| ATOM | 1166 | C | VAL | A | 149 | 39.164 | 23.848 | 56.367 | 1.00 | 21.48 | AAAA |
| ATOM | 1167 | O | VAL | A | 149 | 40.147 | 23.197 | 56.735 | 1.00 | 22.11 | AAAA |
| ATOM | 1168 | N | GLU | A | 150 | 38.628 | 24.826 | 57.088 | 1.00 | 21.19 | AAAA |
| ATOM | 1169 | CA | GLU | A | 150 | 39.171 | 25.176 | 58.386 | 1.00 | 21.70 | AAAA |
| ATOM | 1170 | C | GLU | A | 150 | 38.973 | 24.043 | 59.368 | 1.00 | 22.31 | AAAA |
| ATOM | 1171 | O | GLY | A | 150 | 39.913 | 23.597 | 60.026 | 1.00 | 22.51 | AAAA |
| ATOM | 1172 | N | ILE | A | 151 | 37.736 | 23.566 | 59.453 | 1.00 | 22.86 | AAAA |
| ATOM | 1173 | CA | ILE | A | 151 | 37.388 | 22.474 | 60.346 | 1.00 | 22.26 | AAAA |
| ATOM | 1174 | CB | ILE | A | 151 | 35.894 | 22.124 | 60.191 | 1.00 | 21.51 | AAAA |
| ATOM | 1175 | CG2 | ILE | A | 151 | 35.542 | 20.899 | 61.019 | 1.00 | 21.36 | AAAA |
| ATOM | 1176 | CG1 | ILE | A | 151 | 35.051 | 23.329 | 60.627 | 1.00 | 20.39 | AAAA |
| ATOM | 1177 | CD1 | ILE | A | 151 | 33.576 | 23.199 | 60.361 | 1.00 | 16.88 | AAAA |
| ATOM | 1178 | C | ILE | A | 151 | 38.265 | 21.243 | 60.096 | 1.00 | 23.29 | AAAA |
| ATOM | 1179 | O | ILE | A | 151 | 38.786 | 20.660 | 61.038 | 1.00 | 23.88 | AAAA |
| ATOM | 1180 | N | GLU | A | 152 | 38.435 | 20.853 | 58.836 | 1.00 | 24.13 | AAAA |
| ATOM | 1181 | CA | GLU | A | 152 | 39.267 | 19.697 | 58.517 | 1.00 | 25.01 | AAAA |
| ATOM | 1182 | CB | GLU | A | 152 | 39.242 | 19.404 | 57.010 | 1.00 | 25.07 | AAAA |
| ATOM | 1183 | CG | GLU | A | 152 | 37.910 | 18.886 | 56.526 | 1.00 | 24.56 | AAAA |
| ATOM | 1184 | CD | GLU | A | 152 | 37.500 | 17.570 | 57.198 | 1.00 | 25.00 | AAAA |
| ATOM | 1185 | OE1 | GLU | A | 152 | 36.345 | 17.158 | 57.011 | 1.00 | 26.40 | AAAA |
| ATOM | 1186 | OE2 | GLU | A | 152 | 38.315 | 16.935 | 57.897 | 1.00 | 25.00 | AAAA |
| ATOM | 1187 | C | GLU | A | 152 | 40.694 | 19.957 | 58.965 | 1.00 | 26.06 | AAAA |
| ATOM | 1188 | O | GLU | A | 152 | 41.425 | 19.035 | 59.331 | 1.00 | 26.40 | AAAA |

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Figure 19-19

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1189 | N | TYR | A | 153 | 41.085 | 21.225 | 58.925 | 1.00 | 27.30 | AAAA |
| ATOM | 1190 | CA | TYR | A | 153 | 42.422 | 21.632 | 59.334 | 1.00 | 27.63 | AAAA |
| ATOM | 1191 | CB | TYR | A | 153 | 42.532 | 23.153 | 59.268 | 1.00 | 26.99 | AAAA |
| ATOM | 1192 | CG | TYR | A | 153 | 43.856 | 23.719 | 59.710 | 1.00 | 27.03 | AAAA |
| ATOM | 1193 | CD1 | TYR | A | 153 | 44.942 | 23.790 | 58.837 | 1.00 | 27.78 | AAAA |
| ATOM | 1194 | CE1 | TYR | A | 153 | 46.165 | 24.356 | 59.250 | 1.00 | 28.40 | AAAA |
| ATOM | 1195 | CD2 | TYR | A | 153 | 44.017 | 24.215 | 61.007 | 1.00 | 27.52 | AAAA |
| ATOM | 1196 | CE2 | TYR | A | 153 | 45.216 | 24.774 | 61.425 | 1.00 | 27.66 | AAAA |
| ATOM | 1197 | CZ | TYR | A | 153 | 46.284 | 24.845 | 60.547 | 1.00 | 28.15 | AAAA |
| ATOM | 1198 | OH | TYR | A | 153 | 47.457 | 25.407 | 60.974 | 1.00 | 28.83 | AAAA |
| ATOM | 1199 | C | TYR | A | 153 | 42.618 | 21.172 | 60.769 | 1.00 | 27.82 | AAAA |
| ATOM | 1200 | O | TYR | A | 153 | 43.613 | 20.552 | 61.110 | 1.00 | 27.15 | AAAA |
| ATOM | 1201 | N | LEU | A | 154 | 41.636 | 21.487 | 61.604 | 1.00 | 29.25 | AAAA |
| ATOM | 1202 | CA | LEU | A | 154 | 41.665 | 21.138 | 63.014 | 1.00 | 29.35 | AAAA |
| ATOM | 1203 | CB | LEU | A | 154 | 40.507 | 21.829 | 63.715 | 1.00 | 30.25 | AAAA |
| ATOM | 1204 | CG | LEU | A | 154 | 40.685 | 23.346 | 63.792 | 1.00 | 31.10 | AAAA |
| ATOM | 1205 | CD1 | LEU | A | 154 | 39.348 | 24.020 | 64.092 | 1.00 | 31.24 | AAAA |
| ATOM | 1206 | CD2 | LEU | A | 154 | 41.747 | 23.669 | 64.852 | 1.00 | 29.84 | AAAA |
| ATOM | 1207 | C | LEU | A | 154 | 41.625 | 19.639 | 63.263 | 1.00 | 29.73 | AAAA |
| ATOM | 1208 | O | LEU | A | 154 | 42.313 | 19.151 | 64.150 | 1.00 | 30.51 | AAAA |
| ATOM | 1209 | N | ARG | A | 155 | 40.832 | 18.903 | 62.489 | 1.00 | 28.95 | AAAA |
| ATOM | 1210 | CA | ARG | A | 155 | 40.771 | 17.459 | 62.671 | 1.00 | 28.94 | AAAA |
| ATOM | 1211 | CB | ARG | A | 155 | 39.742 | 16.820 | 61.723 | 1.00 | 28.64 | AAAA |
| ATOM | 1212 | CG | ARG | A | 155 | 38.312 | 17.312 | 61.952 | 1.00 | 27.82 | AAAA |
| ATOM | 1213 | CD | ARG | A | 155 | 37.319 | 16.751 | 60.955 | 1.00 | 27.19 | AAAA |
| ATOM | 1214 | NE | ARG | A | 155 | 36.804 | 15.444 | 61.338 | 1.00 | 28.86 | AAAA |
| ATOM | 1215 | CZ | ARG | A | 155 | 35.939 | 14.742 | 60.612 | 1.00 | 28.93 | AAAA |
| ATOM | 1216 | NH1 | ARG | A | 155 | 35.500 | 15.227 | 59.459 | 1.00 | 29.47 | AAAA |
| ATOM | 1217 | NH2 | ARG | A | 155 | 35.486 | 13.574 | 61.053 | 1.00 | 28.76 | AAAA |
| ATOM | 1218 | C | ARG | A | 155 | 42.158 | 16.853 | 62.438 | 1.00 | 30.20 | AAAA |
| ATOM | 1219 | O | ARG | A | 155 | 42.572 | 15.949 | 63.164 | 1.00 | 30.74 | AAAA |
| ATOM | 1220 | N | LYS | A | 156 | 42.890 | 17.362 | 61.447 | 1.00 | 30.32 | AAAA |
| ATOM | 1221 | CA | LYS | A | 156 | 44.224 | 16.838 | 61.173 | 1.00 | 30.07 | AAAA |
| ATOM | 1222 | CB | LYS | A | 156 | 44.771 | 17.373 | 59.847 | 1.00 | 30.26 | AAAA |
| ATOM | 1223 | CG | LYS | A | 156 | 46.168 | 16.869 | 59.525 | 1.00 | 30.16 | AAAA |
| ATOM | 1224 | CD | LYS | A | 156 | 46.686 | 17.368 | 58.181 | 1.00 | 31.19 | AAAA |
| ATOM | 1225 | CE | LYS | A | 156 | 45.884 | 16.813 | 56.986 | 1.00 | 31.70 | AAAA |
| ATOM | 1226 | NZ | LYS | A | 156 | 45.963 | 15.324 | 56.824 | 1.00 | 31.20 | AAAA |
| ATOM | 1227 | C | LYS | A | 156 | 45.167 | 17.202 | 62.306 | 1.00 | 30.08 | AAAA |
| ATOM | 1228 | O | LYS | A | 156 | 46.192 | 16.550 | 62.485 | 1.00 | 29.16 | AAAA |
| ATOM | 1229 | N | LYS | A | 157 | 44.816 | 18.252 | 63.053 | 1.00 | 30.08 | AAAA |
| ATOM | 1230 | CA | LYS | A | 157 | 45.608 | 18.691 | 64.196 | 1.00 | 31.03 | AAAA |
| ATOM | 1231 | CB | LYS | A | 157 | 45.446 | 20.201 | 64.452 | 1.00 | 31.81 | AAAA |
| ATOM | 1232 | CG | LYS | A | 157 | 46.067 | 21.134 | 63.419 | 1.00 | 32.12 | AAAA |
| ATOM | 1233 | CD | LYS | A | 157 | 47.580 | 21.041 | 63.348 | 1.00 | 31.34 | AAAA |
| ATOM | 1234 | CE | LYS | A | 157 | 48.080 | 21.941 | 62.226 | 1.00 | 32.66 | AAAA |
| ATOM | 1235 | NZ | LYS | A | 157 | 49.556 | 21.921 | 61.996 | 1.00 | 32.74 | AAAA |
| ATOM | 1236 | C | LYS | A | 157 | 45.196 | 17.923 | 65.458 | 1.00 | 31.73 | AAAA |
| ATOM | 1237 | O | LYS | A | 157 | 45.652 | 18.230 | 66.558 | 1.00 | 31.93 | AAAA |
| ATOM | 1238 | N | GLY | A | 158 | 44.312 | 16.942 | 65.299 | 1.00 | 32.41 | AAAA |
| ATOM | 1239 | CA | GLY | A | 158 | 43.901 | 16.140 | 66.436 | 1.00 | 32.34 | AAAA |
| ATOM | 1240 | C | GLY | A | 158 | 42.604 | 16.429 | 67.172 | 1.00 | 32.65 | AAAA |
| ATOM | 1241 | O | GLY | A | 158 | 42.182 | 15.604 | 67.980 | 1.00 | 32.85 | AAAA |
| ATOM | 1242 | N | PHE | A | 159 | 41.960 | 17.565 | 66.932 | 1.00 | 33.16 | AAAA |
| ATOM | 1243 | CA | PHE | A | 159 | 40.712 | 17.842 | 67.650 | 1.00 | 34.16 | AAAA |
| ATOM | 1244 | CB | PHE | A | 159 | 40.220 | 19.281 | 67.403 | 1.00 | 34.81 | AAAA |
| ATOM | 1245 | CG | PHE | A | 159 | 41.134 | 20.343 | 67.965 | 1.00 | 34.01 | AAAA |
| ATOM | 1246 | CD1 | PHE | A | 159 | 42.327 | 20.669 | 67.329 | 1.00 | 34.18 | AAAA |
| ATOM | 1247 | CD2 | PHE | A | 159 | 40.821 | 20.981 | 69.166 | 1.00 | 34.61 | AAAA |
| ATOM | 1248 | CE1 | PHE | A | 159 | 43.197 | 21.610 | 67.874 | 1.00 | 33.65 | AAAA |
| ATOM | 1249 | CE2 | PHE | A | 159 | 41.689 | 21.924 | 69.718 | 1.00 | 34.52 | AAAA |
| ATOM | 1250 | CZ | PHE | A | 159 | 42.878 | 22.236 | 69.065 | 1.00 | 33.90 | AAAA |
| ATOM | 1251 | C | PHE | A | 159 | 39.645 | 16.840 | 67.239 | 1.00 | 34.04 | AAAA |
| ATOM | 1252 | O | PHE | A | 159 | 39.568 | 16.456 | 66.068 | 1.00 | 34.98 | AAAA |
| ATOM | 1253 | N | LYS | A | 160 | 38.839 | 16.403 | 68.202 | 1.00 | 33.36 | AAAA |
| ATOM | 1254 | CA | LYS | A | 160 | 37.794 | 15.415 | 67.936 | 1.00 | 33.11 | AAAA |

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Figure 19-20

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1255 | CB | LYS | A | 160 | 38.060 | 14.140 | 68.763 | 1.00 | 33.97 | AAAA |
| ATOM | 1256 | CG | LYS | A | 160 | 39.410 | 13.491 | 68.457 | 1.00 | 35.31 | AAAA |
| ATOM | 1257 | CD | LYS | A | 160 | 39.833 | 12.364 | 69.429 | 1.00 | 36.48 | AAAA |
| ATOM | 1258 | CE | LYS | A | 160 | 39.095 | 11.037 | 69.243 | 1.00 | 37.97 | AAAA |
| ATOM | 1259 | NZ | LYS | A | 160 | 37.636 | 11.080 | 69.568 | 1.00 | 39.67 | AAAA |
| ATOM | 1260 | C | LYS | A | 160 | 36.385 | 15.941 | 68.210 | 1.00 | 31.68 | AAAA |
| ATOM | 1261 | O | LYS | A | 160 | 35.405 | 15.290 | 67.887 | 1.00 | 31.51 | AAAA |
| ATOM | 1262 | N | ARG | A | 161 | 36.291 | 17.114 | 68.819 | 1.00 | 31.11 | AAAA |
| ATOM | 1263 | CA | ARG | A | 161 | 35.003 | 17.719 | 69.114 | 1.00 | 30.92 | AAAA |
| ATOM | 1264 | CB | ARG | A | 161 | 34.655 | 17.592 | 70.604 | 1.00 | 31.78 | AAAA |
| ATOM | 1265 | CG | ARG | A | 161 | 34.451 | 16.157 | 71.102 | 1.00 | 32.91 | AAAA |
| ATOM | 1266 | CD | ARG | A | 161 | 33.994 | 16.126 | 72.570 | 1.00 | 33.26 | AAAA |
| ATOM | 1267 | NE | ARG | A | 161 | 34.929 | 16.797 | 73.476 | 1.00 | 34.01 | AAAA |
| ATOM | 1268 | CZ | ARG | A | 161 | 36.183 | 16.404 | 73.698 | 1.00 | 34.88 | AAAA |
| ATOM | 1269 | NH1 | ARG | A | 161 | 36.675 | 15.334 | 73.081 | 1.00 | 34.89 | AAAA |
| ATOM | 1270 | NH2 | ARG | A | 161 | 36.954 | 17.084 | 74.537 | 1.00 | 34.71 | AAAA |
| ATOM | 1271 | C | ARG | A | 161 | 35.061 | 19.185 | 68.714 | 1.00 | 30.28 | AAAA |
| ATOM | 1272 | O | ARG | A | 161 | 35.365 | 20.059 | 69.529 | 1.00 | 29.86 | AAAA |
| ATOM | 1273 | N | ILE | A | 162 | 34.774 | 19.433 | 67.437 | 1.00 | 28.86 | AAAA |
| ATOM | 1274 | CA | ILE | A | 162 | 34.788 | 20.774 | 66.862 | 1.00 | 26.41 | AAAA |
| ATOM | 1275 | CB | ILE | A | 162 | 35.443 | 20.762 | 65.464 | 1.00 | 26.87 | AAAA |
| ATOM | 1276 | CG2 | ILE | A | 162 | 35.453 | 22.160 | 64.872 | 1.00 | 26.91 | AAAA |
| ATOM | 1277 | CG1 | ILE | A | 162 | 36.877 | 20.234 | 65.578 | 1.00 | 28.19 | AAAA |
| ATOM | 1278 | CD1 | ILE | A | 162 | 37.614 | 20.090 | 64.240 | 1.00 | 28.24 | AAAA |
| ATOM | 1279 | C | ILE | A | 162 | 33.369 | 21.283 | 66.731 | 1.00 | 24.08 | AAAA |
| ATOM | 1280 | O | ILE | A | 162 | 32.485 | 20.572 | 66.267 | 1.00 | 24.40 | AAAA |
| ATOM | 1281 | N | LEU | A | 163 | 33.153 | 22.519 | 67.153 | 1.00 | 22.25 | AAAA |
| ATOM | 1282 | CA | LEU | A | 163 | 31.838 | 23.126 | 67.074 | 1.00 | 20.48 | AAAA |
| ATOM | 1283 | CB | LEU | A | 163 | 31.408 | 23.671 | 68.440 | 1.00 | 20.97 | AAAA |
| ATOM | 1284 | CG | LEU | A | 163 | 30.099 | 24.477 | 68.486 | 1.00 | 20.50 | AAAA |
| ATOM | 1285 | CD1 | LEU | A | 163 | 28.998 | 23.695 | 67.799 | 1.00 | 19.07 | AAAA |
| ATOM | 1286 | CD2 | LEU | A | 163 | 29.738 | 24.802 | 69.950 | 1.00 | 19.76 | AAAA |
| ATOM | 1287 | C | LEU | A | 163 | 31.801 | 24.241 | 66.055 | 1.00 | 18.76 | AAAA |
| ATOM | 1288 | O | LEU | A | 163 | 32.756 | 24.986 | 65.894 | 1.00 | 18.41 | AAAA |
| ATOM | 1289 | N | TYR | A | 164 | 30.677 | 24.344 | 65.368 | 1.00 | 17.85 | AAAA |
| ATOM | 1290 | CA | TYR | A | 164 | 30.496 | 25.372 | 64.373 | 1.00 | 17.16 | AAAA |
| ATOM | 1291 | CB | TYR | A | 164 | 30.644 | 24.768 | 62.983 | 1.00 | 17.45 | AAAA |
| ATOM | 1292 | CG | TYR | A | 164 | 30.484 | 25.783 | 61.900 | 1.00 | 17.70 | AAAA |
| ATOM | 1293 | CD1 | TYR | A | 164 | 31.444 | 26.772 | 61.701 | 1.00 | 16.23 | AAAA |
| ATOM | 1294 | CE1 | TYR | A | 164 | 31.280 | 27.734 | 60.721 | 1.00 | 17.35 | AAAA |
| ATOM | 1295 | CD2 | TYR | A | 164 | 29.350 | 25.781 | 61.092 | 1.00 | 17.95 | AAAA |
| ATOM | 1296 | CE2 | TYR | A | 164 | 29.173 | 26.746 | 60.103 | 1.00 | 18.03 | AAAA |
| ATOM | 1297 | CZ | TYR | A | 164 | 30.138 | 27.717 | 59.919 | 1.00 | 17.30 | AAAA |
| ATOM | 1298 | OH | TYR | A | 164 | 29.955 | 28.647 | 58.926 | 1.00 | 16.70 | AAAA |
| ATOM | 1299 | C | TYR | A | 164 | 29.123 | 26.016 | 64.514 | 1.00 | 15.85 | AAAA |
| ATOM | 1300 | O | TYR | A | 164 | 28.101 | 25.351 | 64.416 | 1.00 | 16.44 | AAAA |
| ATOM | 1301 | N | ILE | A | 165 | 29.115 | 27.319 | 64.743 | 1.00 | 15.54 | AAAA |
| ATOM | 1302 | CA | ILE | A | 165 | 27.878 | 28.088 | 64.897 | 1.00 | 15.71 | AAAA |
| ATOM | 1303 | CB | ILE | A | 165 | 27.869 | 28.819 | 66.250 | 1.00 | 15.18 | AAAA |
| ATOM | 1304 | CG2 | ILE | A | 165 | 26.621 | 29.685 | 66.374 | 1.00 | 13.94 | AAAA |
| ATOM | 1305 | CG1 | ILE | A | 165 | 28.000 | 27.797 | 67.386 | 1.00 | 13.94 | AAAA |
| ATOM | 1306 | CD1 | ILE | A | 165 | 28.356 | 28.421 | 68.747 | 1.00 | 13.94 | AAAA |
| ATOM | 1307 | C | ILE | A | 165 | 27.808 | 29.124 | 63.754 | 1.00 | 16.00 | AAAA |
| ATOM | 1308 | O | ILE | A | 165 | 28.711 | 29.941 | 63.576 | 1.00 | 16.56 | AAAA |
| ATOM | 1309 | N | ASP | A | 166 | 26.721 | 29.087 | 63.001 | 1.00 | 16.18 | AAAA |
| ATOM | 1310 | CA | ASP | A | 166 | 26.524 | 29.962 | 61.865 | 1.00 | 16.67 | AAAA |
| ATOM | 1311 | CB | ASP | A | 166 | 26.240 | 29.066 | 60.651 | 1.00 | 18.05 | AAAA |
| ATOM | 1312 | CG | ASP | A | 166 | 26.238 | 29.809 | 59.329 | 1.00 | 19.21 | AAAA |
| ATOM | 1313 | OD1 | ASP | A | 166 | 25.353 | 30.659 | 59.114 | 1.00 | 18.36 | AAAA |
| ATOM | 1314 | OD2 | ASP | A | 166 | 27.131 | 29.521 | 58.495 | 1.00 | 19.19 | AAAA |
| ATOM | 1315 | C | ASP | A | 166 | 25.342 | 30.904 | 62.169 | 1.00 | 17.57 | AAAA |
| ATOM | 1316 | O | ASP | A | 166 | 24.206 | 30.459 | 62.321 | 1.00 | 17.26 | AAAA |
| ATOM | 1317 | N | LEU | A | 167 | 25.605 | 32.202 | 62.274 | 1.00 | 16.67 | AAAA |
| ATOM | 1318 | CA | LEU | A | 167 | 24.526 | 33.135 | 62.562 | 1.00 | 16.89 | AAAA |
| ATOM | 1319 | CB | LEU | A | 167 | 24.923 | 34.116 | 63.663 | 1.00 | 17.27 | AAAA |
| ATOM | 1320 | CG | LEU | A | 167 | 25.499 | 33.529 | 64.954 | 1.00 | 18.37 | AAAA |

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Figure 19-21

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1321 | CD1 | LEU | A | 167 | 25.760 | 34.671 | 65.933 | 1.00 | 18.72 | AAAA |
| ATOM | 1322 | CD2 | LEU | A | 167 | 24.566 | 32.507 | 65.547 | 1.00 | 17.06 | AAAA |
| ATOM | 1323 | C | LEU | A | 167 | 24.146 | 33.897 | 61.307 | 1.00 | 17.18 | AAAA |
| ATOM | 1324 | O | LEU | A | 167 | 23.390 | 34.850 | 61.358 | 1.00 | 17.21 | AAAA |
| ATOM | 1325 | N | ASP | A | 168 | 24.683 | 33.457 | 60.178 | 1.00 | 17.83 | AAAA |
| ATOM | 1326 | CA | ASP | A | 168 | 24.382 | 34.067 | 58.904 | 1.00 | 17.84 | AAAA |
| ATOM | 1327 | CB | ASP | A | 168 | 25.178 | 33.397 | 57.807 | 1.00 | 20.42 | AAAA |
| ATOM | 1328 | CG | ASP | A | 168 | 25.140 | 34.162 | 56.529 | 1.00 | 21.41 | AAAA |
| ATOM | 1329 | C | ASP | A | 168 | 22.915 | 33.783 | 58.660 | 1.00 | 18.35 | AAAA |
| ATOM | 1330 | O | ASP | A | 168 | 22.419 | 32.722 | 59.032 | 1.00 | 19.62 | AAAA |
| ATOM | 1331 | OD1 | ASP | A | 168 | 26.066 | 34.972 | 56.330 | 1.00 | 22.42 | AAAA |
| ATOM | 1332 | OD2 | ASP | A | 168 | 24.186 | 33.971 | 55.746 | 1.00 | 21.79 | AAAA |
| ATOM | 1333 | N | ALA | A | 169 | 22.239 | 34.717 | 58.010 | 1.00 | 17.98 | AAAA |
| ATOM | 1334 | CA | ALA | A | 169 | 20.824 | 34.601 | 57.708 | 1.00 | 17.36 | AAAA |
| ATOM | 1335 | CB | ALA | A | 169 | 20.348 | 35.860 | 57.007 | 1.00 | 17.00 | AAAA |
| ATOM | 1336 | C | ALA | A | 169 | 20.439 | 33.377 | 56.887 | 1.00 | 18.64 | AAAA |
| ATOM | 1337 | O | ALA | A | 169 | 19.255 | 33.043 | 56.819 | 1.00 | 19.46 | AAAA |
| ATOM | 1338 | N | HIS | A | 170 | 21.412 | 32.712 | 56.262 | 1.00 | 18.71 | AAAA |
| ATOM | 1339 | CA | HIS | A | 170 | 21.107 | 31.518 | 55.464 | 1.00 | 18.43 | AAAA |
| ATOM | 1340 | C | HIS | A | 170 | 21.802 | 30.265 | 55.986 | 1.00 | 18.02 | AAAA |
| ATOM | 1341 | O | HIS | A | 170 | 22.910 | 30.332 | 56.514 | 1.00 | 17.20 | AAAA |
| ATOM | 1342 | CB | HIS | A | 170 | 21.539 | 31.678 | 54.004 | 1.00 | 18.79 | AAAA |
| ATOM | 1343 | CG | HIS | A | 170 | 21.137 | 32.968 | 53.386 | 1.00 | 17.65 | AAAA |
| ATOM | 1344 | ND1 | HIS | A | 170 | 21.644 | 34.162 | 53.828 | 1.00 | 18.08 | AAAA |
| ATOM | 1345 | CE1 | HIS | A | 170 | 21.112 | 35.081 | 53.054 | 1.00 | 18.95 | AAAA |
| ATOM | 1346 | CD2 | HIS | A | 170 | 20.301 | 33.194 | 52.348 | 1.00 | 18.81 | AAAA |
| ATOM | 1347 | NE2 | HIS | A | 170 | 20.291 | 34.544 | 52.140 | 1.00 | 19.66 | AAAA |
| ATOM | 1348 | N | HIS | A | 171 | 21.142 | 29.124 | 55.793 | 1.00 | 17.53 | AAAA |
| ATOM | 1349 | CA | HIS | A | 171 | 21.662 | 27.822 | 56.193 | 1.00 | 16.38 | AAAA |
| ATOM | 1350 | CB | HIS | A | 171 | 20.644 | 26.740 | 55.830 | 1.00 | 16.32 | AAAA |
| ATOM | 1351 | CG | HIS | A | 171 | 21.157 | 25.337 | 55.958 | 1.00 | 15.91 | AAAA |
| ATOM | 1352 | CD2 | HIS | A | 171 | 21.241 | 24.336 | 55.051 | 1.00 | 14.14 | AAAA |
| ATOM | 1353 | ND1 | HIS | A | 171 | 21.602 | 24.807 | 57.151 | 1.00 | 16.79 | AAAA |
| ATOM | 1354 | CE1 | HIS | A | 171 | 21.937 | 23.543 | 56.973 | 1.00 | 14.91 | AAAA |
| ATOM | 1355 | NE2 | HIS | A | 171 | 21.725 | 23.234 | 55.709 | 1.00 | 15.45 | AAAA |
| ATOM | 1356 | C | HIS | A | 171 | 22.982 | 27.522 | 55.509 | 1.00 | 16.94 | AAAA |
| ATOM | 1357 | O | HIS | A | 171 | 23.146 | 27.725 | 54.318 | 1.00 | 18.71 | AAAA |
| ATOM | 1358 | N | CYS | A | 172 | 23.926 | 27.019 | 56.279 | 1.00 | 16.99 | AAAA |
| ATOM | 1359 | CA | CYS | A | 172 | 25.237 | 26.670 | 55.778 | 1.00 | 16.23 | AAAA |
| ATOM | 1360 | CB | CYS | A | 172 | 26.219 | 26.721 | 56.947 | 1.00 | 17.89 | AAAA |
| ATOM | 1361 | SG | CYS | A | 172 | 25.638 | 25.773 | 58.397 | 1.00 | 17.89 | AAAA |
| ATOM | 1362 | C | CYS | A | 172 | 25.205 | 25.271 | 55.210 | 1.00 | 16.57 | AAAA |
| ATOM | 1363 | O | CYS | A | 172 | 25.947 | 24.413 | 55.670 | 1.00 | 17.66 | AAAA |
| ATOM | 1364 | N | ASP | A | 173 | 24.364 | 25.026 | 54.214 | 1.00 | 18.25 | AAAA |
| ATOM | 1365 | CA | ASP | A | 173 | 24.253 | 23.680 | 53.620 | 1.00 | 19.91 | AAAA |
| ATOM | 1366 | CB | ASP | A | 173 | 23.342 | 23.699 | 52.397 | 1.00 | 20.86 | AAAA |
| ATOM | 1367 | CG | ASP | A | 173 | 23.780 | 24.719 | 51.358 | 1.00 | 21.90 | AAAA |
| ATOM | 1368 | OD1 | ASP | A | 173 | 23.257 | 24.640 | 50.217 | 1.00 | 21.35 | AAAA |
| ATOM | 1369 | OD2 | ASP | A | 173 | 24.624 | 25.597 | 51.687 | 1.00 | 21.35 | AAAA |
| ATOM | 1370 | C | ASP | A | 173 | 25.573 | 23.021 | 53.227 | 1.00 | 21.02 | AAAA |
| ATOM | 1371 | O | ASP | A | 173 | 25.673 | 21.785 | 53.199 | 1.00 | 22.79 | AAAA |
| ATOM | 1372 | N | GLY | A | 174 | 26.579 | 23.832 | 52.912 | 1.00 | 20.03 | AAAA |
| ATOM | 1373 | CA | GLY | A | 174 | 27.870 | 23.277 | 52.553 | 1.00 | 19.72 | AAAA |
| ATOM | 1374 | C | GLY | A | 174 | 28.537 | 22.680 | 53.771 | 1.00 | 20.27 | AAAA |
| ATOM | 1375 | O | GLY | A | 174 | 29.110 | 21.599 | 53.711 | 1.00 | 19.77 | AAAA |
| ATOM | 1376 | N | VAL | A | 175 | 28.448 | 23.387 | 54.893 | 1.00 | 21.38 | AAAA |
| ATOM | 1377 | CA | VAL | A | 175 | 29.056 | 22.934 | 56.135 | 1.00 | 22.26 | AAAA |
| ATOM | 1378 | CB | VAL | A | 175 | 29.032 | 24.040 | 57.203 | 1.00 | 23.15 | AAAA |
| ATOM | 1379 | CG1 | VAL | A | 175 | 29.853 | 23.617 | 58.418 | 1.00 | 22.84 | AAAA |
| ATOM | 1380 | CG2 | VAL | A | 175 | 29.562 | 25.347 | 56.612 | 1.00 | 23.43 | AAAA |
| ATOM | 1381 | C | VAL | A | 175 | 38.302 | 21.724 | 56.654 | 1.00 | 23.51 | AAAA |
| ATOM | 1382 | O | VAL | A | 175 | 28.893 | 20.803 | 57.210 | 1.00 | 23.74 | AAAA |
| ATOM | 1383 | N | GLN | A | 176 | 26.993 | 21.721 | 56.452 | 1.00 | 24.80 | AAAA |
| ATOM | 1384 | CA | GLN | A | 176 | 26.171 | 20.601 | 56.893 | 1.00 | 25.41 | AAAA |
| ATOM | 1385 | CB | GLN | A | 176 | 24.689 | 20.913 | 56.694 | 1.00 | 24.77 | AAAA |
| ATOM | 1386 | CG | GLN | A | 176 | 23.799 | 19.735 | 57.036 | 1.00 | 26.23 | AAAA |

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Figure 19-22

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1387 | CD | GLN | A | 176 | 22.334 | 20.094 | 57.069 | 1.00 | 27.17 | AAAA |
| ATOM | 1388 | OE1 | GLN | A | 176 | 21.902 | 20.879 | 57.911 | 1.00 | 28.24 | AAAA |
| ATOM | 1389 | NE2 | GLN | A | 176 | 21.556 | 19.522 | 56.151 | 1.00 | 26.54 | AAAA |
| ATOM | 1390 | C | GLN | A | 176 | 26.512 | 19.293 | 56.180 | 1.00 | 25.67 | AAAA |
| ATOM | 1391 | O | GLN | A | 176 | 26.789 | 18.285 | 56.820 | 1.00 | 26.98 | AAAA |
| ATOM | 1392 | N | GLU | A | 177 | 26.490 | 19.309 | 54.853 | 1.00 | 26.34 | AAAA |
| ATOM | 1393 | CA | GLU | A | 177 | 26.786 | 18.117 | 54.073 | 1.00 | 26.18 | AAAA |
| ATOM | 1394 | CB | GLU | A | 177 | 26.746 | 18.468 | 52.580 | 1.00 | 27.13 | AAAA |
| ATOM | 1395 | CG | GLU | A | 177 | 26.769 | 17.269 | 51.628 | 1.00 | 29.77 | AAAA |
| ATOM | 1396 | CD | GLU | A | 177 | 26.623 | 17.660 | 50.147 | 1.00 | 31.29 | AAAA |
| ATOM | 1397 | OE1 | GLU | A | 177 | 27.655 | 17.935 | 49.500 | 1.00 | 31.35 | AAAA |
| ATOM | 1398 | OE2 | GLU | A | 177 | 25.471 | 17.703 | 49.636 | 1.00 | 32.05 | AAAA |
| ATOM | 1399 | C | GLU | A | 177 | 28.160 | 17.556 | 54.460 | 1.00 | 26.38 | AAAA |
| ATOM | 1400 | O | GLU | A | 177 | 28.338 | 16.349 | 54.595 | 1.00 | 25.41 | AAAA |
| ATOM | 1401 | N | ALA | A | 178 | 29.115 | 18.458 | 54.659 | 1.00 | 27.58 | AAAA |
| ATOM | 1402 | CA | ALA | A | 178 | 30.495 | 18.119 | 55.004 | 1.00 | 27.66 | AAAA |
| ATOM | 1403 | CB | ALA | A | 178 | 31.345 | 19.385 | 54.994 | 1.00 | 26.20 | AAAA |
| ATOM | 1404 | C | ALA | A | 178 | 30.713 | 17.370 | 56.318 | 1.00 | 28.33 | AAAA |
| ATOM | 1405 | O | ALA | A | 178 | 31.685 | 16.626 | 56.439 | 1.00 | 29.44 | AAAA |
| ATOM | 1406 | N | PHE | A | 179 | 29.849 | 17.564 | 57.308 | 1.00 | 28.25 | AAAA |
| ATOM | 1407 | CA | PHE | A | 179 | 30.036 | 16.852 | 58.561 | 1.00 | 29.20 | AAAA |
| ATOM | 1408 | CB | PHE | A | 179 | 30.570 | 17.794 | 59.624 | 1.00 | 29.35 | AAAA |
| ATOM | 1409 | CG | PHE | A | 179 | 31.751 | 18.572 | 59.171 | 1.00 | 30.26 | AAAA |
| ATOM | 1410 | CD1 | PHE | A | 179 | 31.582 | 19.777 | 58.497 | 1.00 | 31.01 | AAAA |
| ATOM | 1411 | CD2 | PHE | A | 179 | 33.033 | 18.069 | 59.339 | 1.00 | 30.37 | AAAA |
| ATOM | 1412 | CE1 | PHE | A | 179 | 32.670 | 20.470 | 57.993 | 1.00 | 31.20 | AAAA |
| ATOM | 1413 | CE2 | PHE | A | 179 | 34.133 | 18.749 | 58.840 | 1.00 | 31.74 | AAAA |
| ATOM | 1414 | CZ | PHE | A | 179 | 33.950 | 19.960 | 58.161 | 1.00 | 31.81 | AAAA |
| ATOM | 1415 | C | PHE | A | 179 | 28.760 | 16.180 | 59.040 | 1.00 | 30.33 | AAAA |
| ATOM | 1416 | O | PHE | A | 179 | 28.624 | 15.810 | 60.215 | 1.00 | 31.82 | AAAA |
| ATOM | 1417 | N | TYR | A | 180 | 27.842 | 15.994 | 58.105 | 1.00 | 29.18 | AAAA |
| ATOM | 1418 | CA | TYR | A | 180 | 26.564 | 15.379 | 58.389 | 1.00 | 28.99 | AAAA |
| ATOM | 1419 | CB | TYR | A | 180 | 25.725 | 15.343 | 57.123 | 1.00 | 28.30 | AAAA |
| ATOM | 1420 | CG | TYR | A | 180 | 24.244 | 15.422 | 57.384 | 1.00 | 28.27 | AAAA |
| ATOM | 1421 | CD1 | TYR | A | 180 | 23.392 | 14.386 | 57.021 | 1.00 | 27.05 | AAAA |
| ATOM | 1422 | CE1 | TYR | A | 180 | 22.029 | 14.491 | 57.197 | 1.00 | 28.51 | AAAA |
| ATOM | 1423 | CD2 | TYR | A | 180 | 23.686 | 16.573 | 57.942 | 1.00 | 29.34 | AAAA |
| ATOM | 1424 | CE2 | TYR | A | 180 | 22.316 | 16.691 | 58.125 | 1.00 | 29.27 | AAAA |
| ATOM | 1425 | CZ | TYR | A | 180 | 21.495 | 15.645 | 57.746 | 1.00 | 29.33 | AAAA |
| ATOM | 1426 | OH | TYR | A | 180 | 20.141 | 15.775 | 57.893 | 1.00 | 30.83 | AAAA |
| ATOM | 1427 | C | TYR | A | 180 | 26.673 | 13.970 | 58.940 | 1.00 | 28.79 | AAAA |
| ATOM | 1428 | O | TYR | A | 180 | 25.877 | 13.577 | 59.785 | 1.00 | 28.71 | AAAA |
| ATOM | 1429 | N | ASP | A | 181 | 27.662 | 13.214 | 58.472 | 1.00 | 29.03 | AAAA |
| ATOM | 1430 | CA | ASP | A | 181 | 27.813 | 11.828 | 58.914 | 1.00 | 28.49 | AAAA |
| ATOM | 1431 | CB | ASP | A | 181 | 28.140 | 10.930 | 57.715 | 1.00 | 27.59 | AAAA |
| ATOM | 1432 | CG | ASP | A | 181 | 29.548 | 11.122 | 57.229 | 1.00 | 28.82 | AAAA |
| ATOM | 1433 | OD1 | ASP | A | 181 | 29.981 | 12.292 | 57.183 | 1.00 | 29.25 | AAAA |
| ATOM | 1434 | OD2 | ASP | A | 181 | 30.216 | 10.119 | 56.887 | 1.00 | 28.68 | AAAA |
| ATOM | 1435 | C | ASP | A | 181 | 28.863 | 11.631 | 60.009 | 1.00 | 27.67 | AAAA |
| ATOM | 1436 | O | ASP | A | 181 | 29.271 | 10.504 | 60.293 | 1.00 | 27.57 | AAAA |
| ATOM | 1437 | N | THR | A | 182 | 29.308 | 12.713 | 60.628 | 1.00 | 26.27 | AAAA |
| ATOM | 1438 | CA | THR | A | 182 | 30.284 | 12.544 | 61.689 | 1.00 | 26.22 | AAAA |
| ATOM | 1439 | CB | THR | A | 182 | 31.670 | 13.118 | 61.317 | 1.00 | 25.92 | AAAA |
| ATOM | 1440 | OG1 | THR | A | 182 | 32.564 | 12.935 | 62.416 | 1.00 | 25.06 | AAAA |
| ATOM | 1441 | CG2 | THR | A | 182 | 31.577 | 14.594 | 60.974 | 1.00 | 25.25 | AAAA |
| ATOM | 1442 | C | THR | A | 182 | 29.792 | 13.223 | 62.934 | 1.00 | 25.87 | AAAA |
| ATOM | 1443 | O | THR | A | 182 | 28.942 | 14.102 | 62.863 | 1.00 | 26.35 | AAAA |
| ATOM | 1444 | N | ASP | A | 183 | 30.327 | 12.804 | 64.071 | 1.00 | 25.86 | AAAA |
| ATOM | 1445 | CA | ASP | A | 183 | 29.953 | 13.370 | 65.355 | 1.00 | 26.12 | AAAA |
| ATOM | 1446 | CB | ASP | A | 183 | 29.468 | 12.260 | 66.274 | 1.00 | 27.10 | AAAA |
| ATOM | 1447 | CG | ASP | A | 183 | 30.515 | 11.194 | 66.488 | 1.00 | 28.80 | AAAA |
| ATOM | 1448 | OD1 | ASP | A | 183 | 31.063 | 10.691 | 65.480 | 1.00 | 29.78 | AAAA |
| ATOM | 1449 | OD2 | ASP | A | 183 | 30.781 | 10.852 | 67.657 | 1.00 | 29.21 | AAAA |
| ATOM | 1450 | C | ASP | A | 183 | 31.126 | 14.120 | 65.995 | 1.00 | 26.77 | AAAA |
| ATOM | 1451 | O | ASP | A | 183 | 31.034 | 14.566 | 67.146 | 1.00 | 26.65 | AAAA |
| ATOM | 1452 | N | GLN | A | 184 | 32.229 | 14.254 | 65.254 | 1.00 | 26.05 | AAAA |

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Figure 19-23

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1453 | CA | GLN | A | 184 | 33.381 | 14.983 | 65.766 | 1.00 | 25.85 | AAAA |
| ATOM | 1454 | CB | GLN | A | 184 | 34.674 | 14.510 | 65.095 | 1.00 | 26.30 | AAAA |
| ATOM | 1455 | CG | GLN | A | 184 | 34.920 | 13.030 | 65.303 | 1.00 | 27.42 | AAAA |
| ATOM | 1456 | CD | GLN | A | 184 | 36.273 | 12.583 | 64.822 | 1.00 | 28.40 | AAAA |
| ATOM | 1457 | OE1 | GLN | A | 184 | 36.685 | 12.905 | 63.709 | 1.00 | 30.05 | AAAA |
| ATOM | 1458 | NE2 | GLN | A | 184 | 36.970 | 11.816 | 65.651 | 1.00 | 29.24 | AAAA |
| ATOM | 1459 | C | GLN | A | 184 | 33.159 | 16.474 | 65.536 | 1.00 | 25.22 | AAAA |
| ATOM | 1460 | O | GLN | A | 184 | 33.734 | 17.316 | 66.220 | 1.00 | 24.57 | AAAA |
| ATOM | 1461 | N | VAL | A | 185 | 32.290 | 16.791 | 64.584 | 1.00 | 25.17 | AAAA |
| ATOM | 1462 | CA | VAL | A | 185 | 31.975 | 18.182 | 64.291 | 1.00 | 24.49 | AAAA |
| ATOM | 1463 | CB | VAL | A | 185 | 32.324 | 18.563 | 62.832 | 1.00 | 23.20 | AAAA |
| ATOM | 1464 | CG1 | VAL | A | 185 | 32.045 | 20.060 | 62.599 | 1.00 | 19.72 | AAAA |
| ATOM | 1465 | CG2 | VAL | A | 185 | 33.777 | 18.205 | 62.543 | 1.00 | 20.67 | AAAA |
| ATOM | 1466 | C | VAL | A | 185 | 30.494 | 18.421 | 64.501 | 1.00 | 24.81 | AAAA |
| ATOM | 1467 | O | VAL | A | 185 | 29.664 | 17.787 | 63.844 | 1.00 | 27.07 | AAAA |
| ATOM | 1468 | N | PHE | A | 186 | 30.162 | 19.311 | 65.434 | 1.00 | 23.40 | AAAA |
| ATOM | 1469 | CA | PHE | A | 186 | 28.768 | 19.645 | 65.684 | 1.00 | 20.31 | AAAA |
| ATOM | 1470 | CB | PHE | A | 186 | 28.513 | 19.937 | 67.164 | 1.00 | 19.77 | AAAA |
| ATOM | 1471 | CG | PHE | A | 186 | 27.057 | 20.037 | 67.500 | 1.00 | 18.55 | AAAA |
| ATOM | 1472 | CD1 | PHE | A | 186 | 26.359 | 18.918 | 67.945 | 1.00 | 17.70 | AAAA |
| ATOM | 1473 | CD2 | PHE | A | 186 | 26.358 | 21.213 | 67.263 | 1.00 | 17.46 | AAAA |
| ATOM | 1474 | CE1 | PHE | A | 186 | 24.999 | 18.964 | 68.147 | 1.00 | 17.35 | AAAA |
| ATOM | 1475 | CE2 | PHE | A | 186 | 24.997 | 21.271 | 67.459 | 1.00 | 18.83 | AAAA |
| ATOM | 1476 | CZ | PHE | A | 186 | 24.308 | 20.138 | 67.905 | 1.00 | 18.67 | AAAA |
| ATOM | 1477 | C | PHE | A | 186 | 28.464 | 20.911 | 64.895 | 1.00 | 19.18 | AAAA |
| ATOM | 1478 | O | PHE | A | 186 | 29.079 | 21.940 | 65.129 | 1.00 | 18.82 | AAAA |
| ATOM | 1479 | N | VAL | A | 187 | 27.520 | 20.834 | 63.964 | 1.00 | 18.34 | AAAA |
| ATOM | 1480 | CA | VAL | A | 187 | 27.137 | 21.993 | 63.160 | 1.00 | 16.47 | AAAA |
| ATOM | 1481 | CB | VAL | A | 187 | 27.006 | 21.630 | 61.655 | 1.00 | 14.30 | AAAA |
| ATOM | 1482 | CG1 | VAL | A | 187 | 26.628 | 22.869 | 60.828 | 1.00 | 10.34 | AAAA |
| ATOM | 1483 | CG2 | VAL | A | 187 | 28.314 | 21.031 | 61.160 | 1.00 | 12.07 | AAAA |
| ATOM | 1484 | C | VAL | A | 187 | 25.806 | 22.511 | 63.665 | 1.00 | 17.43 | AAAA |
| ATOM | 1485 | O | VAL | A | 187 | 24.852 | 21.746 | 63.792 | 1.00 | 16.95 | AAAA |
| ATOM | 1486 | N | LEU | A | 188 | 25.763 | 23.809 | 63.960 | 1.00 | 18.66 | AAAA |
| ATOM | 1487 | CA | LEU | A | 188 | 24.555 | 24.507 | 64.460 | 1.00 | 20.51 | AAAA |
| ATOM | 1488 | CB | LEU | A | 188 | 24.752 | 24.995 | 65.914 | 1.00 | 21.24 | AAAA |
| ATOM | 1489 | CG | LEU | A | 188 | 23.702 | 26.019 | 66.395 | 1.00 | 20.80 | AAAA |
| ATOM | 1490 | CD1 | LEU | A | 188 | 22.365 | 25.323 | 66.493 | 1.00 | 19.77 | AAAA |
| ATOM | 1491 | CD2 | LEU | A | 188 | 24.085 | 26.627 | 67.750 | 1.00 | 20.63 | AAAA |
| ATOM | 1492 | C | LEU | A | 188 | 24.297 | 25.735 | 63.591 | 1.00 | 20.41 | AAAA |
| ATOM | 1493 | O | LEU | A | 188 | 25.223 | 26.484 | 63.288 | 1.00 | 21.86 | AAAA |
| ATOM | 1494 | N | SER | A | 189 | 23.049 | 25.987 | 63.233 | 1.00 | 19.32 | AAAA |
| ATOM | 1495 | CA | SER | A | 189 | 22.786 | 27.130 | 62.381 | 1.00 | 18.06 | AAAA |
| ATOM | 1496 | CB | SER | A | 189 | 22.970 | 26.715 | 60.906 | 1.00 | 18.54 | AAAA |
| ATOM | 1497 | OG | SER | A | 189 | 22.559 | 27.731 | 59.998 | 1.00 | 17.47 | AAAA |
| ATOM | 1498 | C | SER | A | 189 | 21.418 | 27.751 | 62.554 | 1.00 | 17.90 | AAAA |
| ATOM | 1499 | O | SER | A | 189 | 20.404 | 27.051 | 62.540 | 1.00 | 19.54 | AAAA |
| ATOM | 1500 | N | LEU | A | 190 | 21.386 | 29.067 | 62.722 | 1.00 | 16.97 | AAAA |
| ATOM | 1501 | CA | LEU | A | 190 | 20.117 | 29.772 | 62.797 | 1.00 | 18.49 | AAAA |
| ATOM | 1502 | CB | LEU | A | 190 | 20.097 | 30.865 | 63.886 | 1.00 | 17.78 | AAAA |
| ATOM | 1503 | CG | LEU | A | 190 | 20.534 | 30.600 | 65.337 | 1.00 | 17.10 | AAAA |
| ATOM | 1504 | CD1 | LEU | A | 190 | 19.643 | 31.406 | 66.266 | 1.00 | 15.50 | AAAA |
| ATOM | 1505 | CD2 | LEU | A | 190 | 20.455 | 29.147 | 65.686 | 1.00 | 15.15 | AAAA |
| ATOM | 1506 | C | LEU | A | 190 | 20.111 | 30.408 | 61.416 | 1.00 | 19.35 | AAAA |
| ATOM | 1507 | O | LEU | A | 190 | 21.136 | 30.891 | 60.967 | 1.00 | 19.75 | AAAA |
| ATOM | 1508 | N | HIS | A | 191 | 18.975 | 30.397 | 60.736 | 1.00 | 21.75 | AAAA |
| ATOM | 1509 | CA | HIS | A | 191 | 18.897 | 30.955 | 59.383 | 1.00 | 23.55 | AAAA |
| ATOM | 1510 | CB | HIS | A | 191 | 19.626 | 30.013 | 58.426 | 1.00 | 23.63 | AAAA |
| ATOM | 1511 | CG | HIS | A | 191 | 19.157 | 28.597 | 58.533 | 1.00 | 24.26 | AAAA |
| ATOM | 1512 | CD2 | HIS | A | 191 | 19.770 | 27.485 | 59.009 | 1.00 | 23.78 | AAAA |
| ATOM | 1513 | ND1 | HIS | A | 191 | 17.869 | 28.217 | 58.217 | 1.00 | 24.73 | AAAA |
| ATOM | 1514 | CE1 | HIS | A | 191 | 17.709 | 26.935 | 58.491 | 1.00 | 23.90 | AAAA |
| ATOM | 1515 | NE2 | HIS | A | 191 | 18.849 | 26.467 | 58.973 | 1.00 | 24.51 | AAAA |
| ATOM | 1516 | C | HIS | A | 191 | 17.446 | 31.119 | 58.926 | 1.00 | 24.10 | AAAA |
| ATOM | 1517 | O | HIS | A | 191 | 16.519 | 30.658 | 59.596 | 1.00 | 24.94 | AAAA |
| ATOM | 1518 | N | GLN | A | 192 | 17.249 | 31.789 | 57.794 | 1.00 | 24.33 | AAAA |

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Figure 19-24

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1519 | CA | GLN | A | 192 | 15.899 | 31.959 | 57.269 | 1.00 | 25.77 | AAAA |
| ATOM | 1520 | CB | GLN | A | 192 | 15.881 | 32.896 | 56.060 | 1.00 | 26.51 | AAAA |
| ATOM | 1521 | CG | GLN | A | 192 | 16.467 | 34.271 | 56.325 | 1.00 | 26.99 | AAAA |
| ATOM | 1522 | CD | GLN | A | 192 | 16.581 | 35.076 | 55.062 | 1.00 | 27.98 | AAAA |
| ATOM | 1523 | OE1 | GLN | A | 192 | 15.583 | 35.496 | 54.493 | 1.00 | 30.48 | AAAA |
| ATOM | 1524 | NE2 | GLN | A | 192 | 17.802 | 35.274 | 54.595 | 1.00 | 29.04 | AAAA |
| ATOM | 1525 | C | GLN | A | 192 | 15.463 | 30.573 | 56.832 | 1.00 | 25.77 | AAAA |
| ATOM | 1526 | O | GLN | A | 192 | 16.211 | 29.865 | 56.169 | 1.00 | 26.73 | AAAA |
| ATOM | 1527 | N | SER | A | 193 | 14.259 | 30.184 | 57.214 | 1.00 | 25.48 | AAAA |
| ATOM | 1528 | CA | SER | A | 193 | 13.750 | 28.877 | 56.863 | 1.00 | 24.51 | AAAA |
| ATOM | 1529 | CB | SER | A | 193 | 12.288 | 28.788 | 57.286 | 1.00 | 23.77 | AAAA |
| ATOM | 1530 | OG | SER | A | 193 | 11.753 | 27.517 | 57.010 | 1.00 | 24.81 | AAAA |
| ATOM | 1531 | C | SER | A | 193 | 13.906 | 28.597 | 55.361 | 1.00 | 24.53 | AAAA |
| ATOM | 1532 | O | SER | A | 193 | 13.736 | 29.479 | 54.522 | 1.00 | 22.32 | AAAA |
| ATOM | 1533 | N | PRO | A | 194 | 14.226 | 27.348 | 55.007 | 1.00 | 25.69 | AAAA |
| ATOM | 1534 | CD | PRO | A | 194 | 14.411 | 26.167 | 55.862 | 1.00 | 25.02 | AAAA |
| ATOM | 1535 | CA | PRO | A | 194 | 14.399 | 26.976 | 53.604 | 1.00 | 27.05 | AAAA |
| ATOM | 1536 | CB | PRO | A | 194 | 14.906 | 25.535 | 53.697 | 1.00 | 26.30 | AAAA |
| ATOM | 1537 | CG | PRO | A | 194 | 15.479 | 25.466 | 55.124 | 1.00 | 26.44 | AAAA |
| ATOM | 1538 | C | PRO | A | 194 | 13.076 | 27.057 | 52.849 | 1.00 | 27.79 | AAAA |
| ATOM | 1539 | O | PRO | A | 194 | 13.066 | 27.057 | 51.625 | 1.00 | 28.82 | AAAA |
| ATOM | 1540 | N | GLU | A | 195 | 11.966 | 27.133 | 53.582 | 1.00 | 28.29 | AAAA |
| ATOM | 1541 | CA | GLU | A | 195 | 10.656 | 27.187 | 52.950 | 1.00 | 29.08 | AAAA |
| ATOM | 1542 | CB | GLU | A | 195 | 9.534 | 27.030 | 54.001 | 1.00 | 31.08 | AAAA |
| ATOM | 1543 | CG | GLU | A | 195 | 9.070 | 28.294 | 54.722 | 1.00 | 35.07 | AAAA |
| ATOM | 1544 | CD | GLU | A | 195 | 7.850 | 28.980 | 54.064 | 1.00 | 38.05 | AAAA |
| ATOM | 1545 | OE1 | GLU | A | 195 | 7.389 | 30.017 | 54.601 | 1.00 | 38.80 | AAAA |
| ATOM | 1546 | OE2 | GLU | A | 195 | 7.342 | 28.487 | 53.024 | 1.00 | 39.20 | AAAA |
| ATOM | 1547 | C | GLU | A | 195 | 10.483 | 28.471 | 52.150 | 1.00 | 28.05 | AAAA |
| ATOM | 1548 | O | GLU | A | 195 | 9.722 | 28.512 | 51.189 | 1.00 | 28.57 | AAAA |
| ATOM | 1549 | N | TYR | A | 196 | 11.223 | 29.510 | 52.514 | 1.00 | 27.39 | AAAA |
| ATOM | 1550 | CA | TYR | A | 196 | 11.108 | 30.769 | 51.802 | 1.00 | 25.80 | AAAA |
| ATOM | 1551 | CB | TYR | A | 196 | 10.275 | 31.743 | 52.645 | 1.00 | 24.97 | AAAA |
| ATOM | 1552 | CG | TYR | A | 196 | 10.971 | 32.281 | 53.868 | 1.00 | 23.41 | AAAA |
| ATOM | 1553 | CD1 | TYR | A | 196 | 11.911 | 33.306 | 53.765 | 1.00 | 23.99 | AAAA |
| ATOM | 1554 | CE1 | TYR | A | 196 | 12.559 | 33.805 | 54.892 | 1.00 | 23.44 | AAAA |
| ATOM | 1555 | CD2 | TYR | A | 196 | 10.697 | 31.768 | 55.126 | 1.00 | 23.24 | AAAA |
| ATOM | 1556 | CE2 | TYR | A | 196 | 11.336 | 32.256 | 56.254 | 1.00 | 23.93 | AAAA |
| ATOM | 1557 | CZ | TYR | A | 196 | 12.265 | 33.270 | 56.133 | 1.00 | 24.07 | AAAA |
| ATOM | 1558 | OH | TYR | A | 196 | 12.913 | 33.731 | 57.247 | 1.00 | 25.06 | AAAA |
| ATOM | 1559 | C | TYR | A | 196 | 12.450 | 31.406 | 51.411 | 1.00 | 24.97 | AAAA |
| ATOM | 1560 | O | TYR | A | 196 | 12.475 | 32.495 | 50.840 | 1.00 | 25.14 | AAAA |
| ATOM | 1561 | N | ALA | A | 197 | 13.563 | 30.737 | 51.686 | 1.00 | 23.81 | AAAA |
| ATOM | 1562 | CA | ALA | A | 197 | 14.855 | 31.330 | 51.337 | 1.00 | 23.32 | AAAA |
| ATOM | 1563 | CB | ALA | A | 197 | 15.350 | 32.220 | 52.488 | 1.00 | 23.33 | AAAA |
| ATOM | 1564 | C | ALA | A | 197 | 15.952 | 30.356 | 50.957 | 1.00 | 22.74 | AAAA |
| ATOM | 1565 | O | ALA | A | 197 | 15.951 | 29.207 | 51.371 | 1.00 | 22.47 | AAAA |
| ATOM | 1566 | N | PHE | A | 198 | 16.900 | 30.852 | 50.167 | 1.00 | 23.23 | AAAA |
| ATOM | 1567 | CA | PHE | A | 198 | 18.062 | 30.081 | 49.741 | 1.00 | 23.68 | AAAA |
| ATOM | 1568 | CB | PHE | A | 198 | 19.083 | 31.006 | 49.069 | 1.00 | 23.33 | AAAA |
| ATOM | 1569 | CG | PHE | A | 198 | 20.250 | 30.280 | 48.464 | 1.00 | 22.98 | AAAA |
| ATOM | 1570 | CD1 | PHE | A | 198 | 20.151 | 29.713 | 47.203 | 1.00 | 22.75 | AAAA |
| ATOM | 1571 | CD2 | PHE | A | 198 | 21.436 | 30.127 | 49.175 | 1.00 | 23.32 | AAAA |
| ATOM | 1572 | CE1 | PHE | A | 198 | 21.207 | 29.003 | 46.645 | 1.00 | 22.13 | AAAA |
| ATOM | 1573 | CE2 | PHE | A | 198 | 22.512 | 29.408 | 48.622 | 1.00 | 22.83 | AAAA |
| ATOM | 1574 | CZ | PHE | A | 198 | 22.386 | 28.849 | 47.351 | 1.00 | 22.55 | AAAA |
| ATOM | 1575 | C | PHE | A | 198 | 18.689 | 29.490 | 51.008 | 1.00 | 23.69 | AAAA |
| ATOM | 1576 | O | PHE | A | 198 | 18.802 | 30.171 | 52.012 | 1.00 | 22.85 | AAAA |
| ATOM | 1577 | N | PRO | A | 199 | 19.166 | 28.236 | 50.954 | 1.00 | 23.96 | AAAA |
| ATOM | 1578 | CD | PRO | A | 199 | 19.833 | 27.639 | 52.123 | 1.00 | 24.26 | AAAA |
| ATOM | 1579 | CA | PRO | A | 199 | 19.199 | 27.286 | 49.837 | 1.00 | 24.70 | AAAA |
| ATOM | 1580 | CB | PRO | A | 199 | 20.163 | 26.222 | 50.357 | 1.00 | 23.30 | AAAA |
| ATOM | 1581 | CG | PRO | A | 199 | 19.797 | 26.162 | 51.782 | 1.00 | 23.21 | AAAA |
| ATOM | 1582 | C | PRO | A | 199 | 17.885 | 26.679 | 49.326 | 1.00 | 25.22 | AAAA |
| ATOM | 1583 | O | PRO | A | 199 | 17.866 | 26.145 | 48.215 | 1.00 | 26.24 | AAAA |
| ATOM | 1584 | N | PHE | A | 200 | 16.811 | 26.756 | 50.116 | 1.00 | 25.09 | AAAA |

SUBSTITUTE SHEET (RULE 26)

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Figure 19-25

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1585 | CA | PHE | A | 200 | 15.497 | 26.190 | 49.763 | 1.00 | 26.29 | AAAA |
| ATOM | 1586 | CB | PHE | A | 200 | 15.064 | 26.567 | 48.340 | 1.00 | 25.65 | AAAA |
| ATOM | 1587 | CG | PHE | A | 200 | 14.863 | 28.035 | 48.122 | 1.00 | 24.65 | AAAA |
| ATOM | 1588 | CD1 | PHE | A | 200 | 15.806 | 28.781 | 47.439 | 1.00 | 24.42 | AAAA |
| ATOM | 1589 | CD2 | PHE | A | 200 | 13.735 | 28.671 | 48.608 | 1.00 | 23.79 | AAAA |
| ATOM | 1590 | CE1 | PHE | A | 200 | 15.631 | 30.125 | 47.246 | 1.00 | 24.41 | AAAA |
| ATOM | 1591 | CE2 | PHE | A | 200 | 13.552 | 30.035 | 48.418 | 1.00 | 24.94 | AAAA |
| ATOM | 1592 | CZ | PHE | A | 200 | 14.499 | 30.760 | 47.738 | 1.00 | 24.57 | AAAA |
| ATOM | 1593 | C | PHE | A | 200 | 15.415 | 24.656 | 49.863 | 1.00 | 28.54 | AAAA |
| ATOM | 1594 | O | PHE | A | 200 | 14.386 | 24.096 | 50.251 | 1.00 | 28.76 | AAAA |
| ATOM | 1595 | N | GLU | A | 201 | 16.499 | 23.981 | 49.504 | 1.00 | 29.67 | AAAA |
| ATOM | 1596 | CA | GLU | A | 201 | 16.539 | 22.528 | 49.524 | 1.00 | 31.88 | AAAA |
| ATOM | 1597 | CB | GLU | A | 201 | 17.434 | 22.045 | 48.392 | 1.00 | 32.71 | AAAA |
| ATOM | 1598 | CG | GLU | A | 201 | 16.897 | 22.415 | 47.017 | 1.00 | 34.87 | AAAA |
| ATOM | 1599 | CD | GLU | A | 201 | 17.898 | 22.147 | 45.912 | 1.00 | 35.14 | AAAA |
| ATOM | 1600 | OE1 | GLU | A | 201 | 18.299 | 20.982 | 45.735 | 1.00 | 36.09 | AAAA |
| ATOM | 1601 | OE2 | GLU | A | 201 | 18.286 | 23.112 | 45.221 | 1.00 | 36.30 | AAAA |
| ATOM | 1602 | C | GLU | A | 201 | 16.997 | 21.894 | 50.835 | 1.00 | 32.77 | AAAA |
| ATOM | 1603 | O | GLU | A | 201 | 16.806 | 20.690 | 51.046 | 1.00 | 33.44 | AAAA |
| ATOM | 1604 | N | LYS | A | 202 | 17.599 | 22.690 | 51.711 | 1.00 | 32.31 | AAAA |
| ATOM | 1605 | CA | LYS | A | 202 | 18.101 | 22.168 | 52.974 | 1.00 | 32.09 | AAAA |
| ATOM | 1606 | CB | LYS | A | 202 | 19.565 | 21.750 | 52.811 | 1.00 | 33.02 | AAAA |
| ATOM | 1607 | CG | LYS | A | 202 | 19.836 | 20.847 | 51.623 | 1.00 | 34.95 | AAAA |
| ATOM | 1608 | CD | LYS | A | 202 | 21.334 | 20.619 | 51.436 | 1.00 | 37.92 | AAAA |
| ATOM | 1609 | CE | LYS | A | 202 | 21.655 | 19.804 | 50.169 | 1.00 | 39.19 | AAAA |
| ATOM | 1610 | NZ | LYS | A | 202 | 23.120 | 19.522 | 49.988 | 1.00 | 38.58 | AAAA |
| ATOM | 1611 | C | LYS | A | 202 | 17.995 | 23.241 | 54.037 | 1.00 | 30.85 | AAAA |
| ATOM | 1612 | O | LYS | A | 202 | 17.706 | 24.389 | 53.739 | 1.00 | 30.49 | AAAA |
| ATOM | 1613 | N | GLY | A | 203 | 18.238 | 22.867 | 55.281 | 1.00 | 30.81 | AAAA |
| ATOM | 1614 | CA | GLY | A | 203 | 18.159 | 23.831 | 56.356 | 1.00 | 30.86 | AAAA |
| ATOM | 1615 | C | GLY | A | 203 | 16.991 | 23.578 | 57.280 | 1.00 | 30.84 | AAAA |
| ATOM | 1616 | O | GLY | A | 203 | 16.828 | 24.285 | 58.272 | 1.00 | 31.58 | AAAA |
| ATOM | 1617 | N | PHE | A | 204 | 16.182 | 22.570 | 56.965 | 1.00 | 30.54 | AAAA |
| ATOM | 1618 | CA | PHE | A | 204 | 15.025 | 22.241 | 57.797 | 1.00 | 30.51 | AAAA |
| ATOM | 1619 | CB | PHE | A | 204 | 14.061 | 21.317 | 57.058 | 1.00 | 29.06 | AAAA |
| ATOM | 1620 | CG | PHE | A | 204 | 13.524 | 21.890 | 55.787 | 1.00 | 27.13 | AAAA |
| ATOM | 1621 | CD1 | PHE | A | 204 | 14.222 | 21.762 | 54.601 | 1.00 | 26.52 | AAAA |
| ATOM | 1622 | CD2 | PHE | A | 204 | 12.307 | 22.548 | 55.779 | 1.00 | 26.50 | AAAA |
| ATOM | 1623 | CE1 | PHE | A | 204 | 13.713 | 22.276 | 53.420 | 1.00 | 26.44 | AAAA |
| ATOM | 1624 | CE2 | PHE | A | 204 | 11.786 | 23.069 | 54.600 | 1.00 | 26.69 | AAAA |
| ATOM | 1625 | CZ | PHE | A | 204 | 12.490 | 22.931 | 53.416 | 1.00 | 25.65 | AAAA |
| ATOM | 1626 | C | PHE | A | 204 | 15.401 | 21.590 | 59.127 | 1.00 | 30.87 | AAAA |
| ATOM | 1627 | O | PHE | A | 204 | 16.395 | 20.875 | 59.228 | 1.00 | 31.12 | AAAA |
| ATOM | 1628 | N | LEU | A | 205 | 14.580 | 21.844 | 60.139 | 1.00 | 31.22 | AAAA |
| ATOM | 1629 | CA | LEU | A | 205 | 14.782 | 21.329 | 61.489 | 1.00 | 31.43 | AAAA |
| ATOM | 1630 | CB | LEU | A | 205 | 13.575 | 21.691 | 62.357 | 1.00 | 31.42 | AAAA |
| ATOM | 1631 | CG | LEU | A | 205 | 13.603 | 21.078 | 63.755 | 1.00 | 31.76 | AAAA |
| ATOM | 1632 | CD1 | LEU | A | 205 | 14.894 | 21.492 | 64.457 | 1.00 | 32.36 | AAAA |
| ATOM | 1633 | CD2 | LEU | A | 205 | 12.379 | 21.516 | 64.536 | 1.00 | 31.31 | AAAA |
| ATOM | 1634 | C | LEU | A | 205 | 15.026 | 19.829 | 61.625 | 1.00 | 31.35 | AAAA |
| ATOM | 1635 | O | LEU | A | 205 | 15.714 | 19.392 | 62.546 | 1.00 | 31.40 | AAAA |
| ATOM | 1636 | N | GLU | A | 206 | 14.448 | 19.059 | 60.707 | 1.00 | 31.79 | AAAA |
| ATOM | 1637 | CA | GLU | A | 206 | 14.509 | 17.603 | 60.706 | 1.00 | 32.08 | AAAA |
| ATOM | 1638 | CB | GLU | A | 206 | 13.485 | 17.054 | 59.716 | 1.00 | 33.18 | AAAA |
| ATOM | 1639 | CG | GLU | A | 206 | 12.069 | 17.651 | 59.829 | 1.00 | 34.20 | AAAA |
| ATOM | 1640 | CD | GLU | A | 206 | 11.973 | 19.136 | 59.453 | 1.00 | 33.44 | AAAA |
| ATOM | 1641 | OE1 | GLU | A | 206 | 10.854 | 19.675 | 59.422 | 1.00 | 33.32 | AAAA |
| ATOM | 1642 | OE2 | GLU | A | 206 | 13.005 | 19.777 | 59.194 | 1.00 | 35.12 | AAAA |
| ATOM | 1643 | C | GLU | A | 206 | 15.882 | 17.045 | 60.363 | 1.00 | 32.34 | AAAA |
| ATOM | 1644 | O | GLU | A | 206 | 16.209 | 15.909 | 60.706 | 1.00 | 31.83 | AAAA |
| ATOM | 1645 | N | GLU | A | 207 | 16.680 | 17.847 | 59.670 | 1.00 | 32.48 | AAAA |
| ATOM | 1646 | CA | GLU | A | 207 | 18.017 | 17.431 | 59.287 | 1.00 | 31.67 | AAAA |
| ATOM | 1647 | CB | GLU | A | 207 | 18.552 | 18.385 | 58.238 | 1.00 | 30.39 | AAAA |
| ATOM | 1648 | CG | GLU | A | 207 | 17.768 | 18.316 | 56.960 | 1.00 | 29.63 | AAAA |
| ATOM | 1649 | CD | GLU | A | 207 | 17.953 | 19.547 | 56.121 | 1.00 | 30.04 | AAAA |
| ATOM | 1650 | OE1 | GLU | A | 207 | 19.108 | 19.991 | 55.971 | 1.00 | 30.31 | AAAA |

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Figure 19-26

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1651 | OE2 | GLU | A | 207 | 16.947 | 20.070 | 55.604 | 1.00 | 30.76 | AAAA |
| ATOM | 1652 | C | GLU | A | 207 | 18.879 | 17.433 | 60.537 | 1.00 | 32.04 | AAAA |
| ATOM | 1653 | O | GLU | A | 207 | 19.472 | 18.448 | 60.910 | 1.00 | 31.57 | AAAA |
| ATOM | 1654 | N | ILE | A | 208 | 18.935 | 16.272 | 61.178 | 1.00 | 32.57 | AAAA |
| ATOM | 1655 | CA | ILE | A | 208 | 19.674 | 16.111 | 62.408 | 1.00 | 33.37 | AAAA |
| ATOM | 1656 | CB | ILE | A | 208 | 18.709 | 15.647 | 63.519 | 1.00 | 33.65 | AAAA |
| ATOM | 1657 | CG2 | ILE | A | 208 | 19.443 | 15.380 | 64.806 | 1.00 | 34.11 | AAAA |
| ATOM | 1658 | CG1 | ILE | A | 208 | 17.673 | 16.742 | 63.757 | 1.00 | 33.94 | AAAA |
| ATOM | 1659 | CD1 | ILE | A | 208 | 16.628 | 16.386 | 64.794 | 1.00 | 37.00 | AAAA |
| ATOM | 1660 | C | ILE | A | 208 | 20.863 | 15.174 | 62.280 | 1.00 | 34.00 | AAAA |
| ATOM | 1661 | O | ILE | A | 208 | 21.506 | 14.829 | 63.265 | 1.00 | 34.40 | AAAA |
| ATOM | 1662 | N | GLY | A | 209 | 21.177 | 14.768 | 61.062 | 1.00 | 34.64 | AAAA |
| ATOM | 1663 | CA | GLY | A | 209 | 22.321 | 13.903 | 60.913 | 1.00 | 35.55 | AAAA |
| ATOM | 1664 | C | GLY | A | 209 | 22.164 | 12.671 | 60.057 | 1.00 | 36.80 | AAAA |
| ATOM | 1665 | O | GLY | A | 209 | 21.148 | 12.461 | 59.400 | 1.00 | 37.32 | AAAA |
| ATOM | 1666 | N | GLU | A | 210 | 23.199 | 11.836 | 60.100 | 1.00 | 37.78 | AAAA |
| ATOM | 1667 | CA | GLU | A | 210 | 23.256 | 10.621 | 59.315 | 1.00 | 38.04 | AAAA |
| ATOM | 1668 | CB | GLU | A | 210 | 23.600 | 11.013 | 57.892 | 1.00 | 38.54 | AAAA |
| ATOM | 1669 | CG | GLU | A | 210 | 23.469 | 9.960 | 56.858 | 1.00 | 38.99 | AAAA |
| ATOM | 1670 | CD | GLU | A | 210 | 24.118 | 10.412 | 55.580 | 1.00 | 40.10 | AAAA |
| ATOM | 1671 | OE1 | GLU | A | 210 | 25.365 | 10.437 | 55.555 | 1.00 | 40.86 | AAAA |
| ATOM | 1672 | OE2 | GLU | A | 210 | 23.396 | 10.767 | 54.619 | 1.00 | 40.41 | AAAA |
| ATOM | 1673 | C | GLU | A | 210 | 24.377 | 9.770 | 59.894 | 1.00 | 37.98 | AAAA |
| ATOM | 1674 | O | GLU | A | 210 | 25.498 | 10.244 | 60.041 | 1.00 | 38.52 | AAAA |
| ATOM | 1675 | N | GLY | A | 211 | 24.085 | 8.517 | 60.220 | 1.00 | 38.02 | AAAA |
| ATOM | 1676 | CA | GLY | A | 211 | 25.116 | 7.654 | 60.770 | 1.00 | 38.09 | AAAA |
| ATOM | 1677 | C | GLY | A | 211 | 25.542 | 8.075 | 62.164 | 1.00 | 38.26 | AAAA |
| ATOM | 1678 | O | GLY | A | 211 | 24.697 | 8.443 | 62.977 | 1.00 | 37.82 | AAAA |
| ATOM | 1679 | N | LYS | A | 212 | 26.848 | 8.030 | 62.434 | 1.00 | 38.20 | AAAA |
| ATOM | 1680 | CA | LYS | A | 212 | 27.396 | 8.399 | 63.743 | 1.00 | 37.56 | AAAA |
| ATOM | 1681 | CB | LYS | A | 212 | 28.921 | 8.209 | 63.766 | 1.00 | 38.86 | AAAA |
| ATOM | 1682 | CG | LYS | A | 212 | 29.416 | 6.810 | 63.385 | 1.00 | 40.93 | AAAA |
| ATOM | 1683 | CD | LYS | A | 212 | 29.001 | 5.746 | 64.405 | 1.00 | 42.04 | AAAA |
| ATOM | 1684 | CE | LYS | A | 212 | 29.251 | 4.318 | 63.891 | 1.00 | 42.80 | AAAA |
| ATOM | 1685 | NZ | LYS | A | 212 | 30.673 | 4.002 | 63.562 | 1.00 | 42.32 | AAAA |
| ATOM | 1686 | C | LYS | A | 212 | 27.093 | 9.859 | 64.054 | 1.00 | 37.08 | AAAA |
| ATOM | 1687 | O | LYS | A | 212 | 27.075 | 10.269 | 65.218 | 1.00 | 36.94 | AAAA |
| ATOM | 1688 | N | GLY | A | 213 | 26.854 | 10.636 | 63.002 | 1.00 | 35.41 | AAAA |
| ATOM | 1689 | CA | GLY | A | 213 | 26.592 | 12.054 | 63.170 | 1.00 | 34.24 | AAAA |
| ATOM | 1690 | C | GLY | A | 213 | 25.163 | 12.438 | 63.470 | 1.00 | 33.27 | AAAA |
| ATOM | 1691 | O | GLY | A | 213 | 24.861 | 13.611 | 63.666 | 1.00 | 33.29 | AAAA |
| ATOM | 1692 | N | LYS | A | 214 | 24.280 | 11.451 | 63.512 | 1.00 | 31.79 | AAAA |
| ATOM | 1693 | CA | LYS | A | 214 | 22.883 | 11.710 | 63.794 | 1.00 | 30.47 | AAAA |
| ATOM | 1694 | CB | LYS | A | 214 | 22.111 | 10.396 | 63.737 | 1.00 | 30.35 | AAAA |
| ATOM | 1695 | CG | LYS | A | 214 | 20.676 | 10.552 | 63.280 | 1.00 | 30.45 | AAAA |
| ATOM | 1696 | CD | LYS | A | 214 | 20.141 | 9.241 | 62.759 | 1.00 | 29.75 | AAAA |
| ATOM | 1697 | CE | LYS | A | 214 | 18.737 | 9.400 | 62.229 | 1.00 | 30.19 | AAAA |
| ATOM | 1698 | NZ | LYS | A | 214 | 18.179 | 8.138 | 61.671 | 1.00 | 31.35 | AAAA |
| ATOM | 1699 | C | LYS | A | 214 | 22.778 | 12.374 | 65.168 | 1.00 | 30.31 | AAAA |
| ATOM | 1700 | O | LYS | A | 214 | 23.193 | 11.814 | 66.177 | 1.00 | 30.44 | AAAA |
| ATOM | 1701 | N | GLY | A | 215 | 22.243 | 13.590 | 65.192 | 1.00 | 29.95 | AAAA |
| ATOM | 1702 | CA | GLY | A | 215 | 22.128 | 14.325 | 66.437 | 1.00 | 29.16 | AAAA |
| ATOM | 1703 | C | GLY | A | 215 | 23.222 | 15.379 | 66.582 | 1.00 | 28.54 | AAAA |
| ATOM | 1704 | O | GLY | A | 215 | 23.306 | 16.061 | 67.602 | 1.00 | 28.27 | AAAA |
| ATOM | 1705 | N | TYR | A | 216 | 24.063 | 15.521 | 65.561 | 1.00 | 27.35 | AAAA |
| ATOM | 1706 | CA | TYR | A | 216 | 25.150 | 16.497 | 65.616 | 1.00 | 27.08 | AAAA |
| ATOM | 1707 | CB | TYR | A | 216 | 26.516 | 15.800 | 65.531 | 1.00 | 28.38 | AAAA |
| ATOM | 1708 | CG | TYR | A | 216 | 26.786 | 14.966 | 66.757 | 1.00 | 30.21 | AAAA |
| ATOM | 1709 | CD1 | TYR | A | 216 | 26.138 | 13.735 | 66.955 | 1.00 | 29.81 | AAAA |
| ATOM | 1710 | CE1 | TYR | A | 216 | 26.311 | 13.014 | 68.138 | 1.00 | 30.03 | AAAA |
| ATOM | 1711 | CD2 | TYR | A | 216 | 27.619 | 15.450 | 67.774 | 1.00 | 29.71 | AAAA |
| ATOM | 1712 | CE2 | TYR | A | 216 | 27.798 | 14.741 | 68.957 | 1.00 | 29.96 | AAAA |
| ATOM | 1713 | CZ | TYR | A | 216 | 27.143 | 13.528 | 69.138 | 1.00 | 30.84 | AAAA |
| ATOM | 1714 | OH | TYR | A | 216 | 27.297 | 12.859 | 70.332 | 1.00 | 31.14 | AAAA |
| ATOM | 1715 | C | TYR | A | 216 | 25.055 | 17.599 | 64.581 | 1.00 | 25.40 | AAAA |
| ATOM | 1716 | O | TYR | A | 216 | 26.046 | 18.240 | 64.243 | 1.00 | 26.38 | AAAA |

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Figure 19-27

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|------|
| ATOM | 1717 | N | ASN A 217 | 23.845 | 17.791 | 64.076 | 1.00 | 23.55 | AAAA |
| ATOM | 1718 | CA | ASN A 217 | 23.549 | 18.830 | 63.119 | 1.00 | 21.52 | AAAA |
| ATOM | 1719 | CB | ASN A 217 | 23.431 | 18.282 | 61.699 | 1.00 | 20.64 | AAAA |
| ATOM | 1720 | CG | ASN A 217 | 23.202 | 19.386 | 60.669 | 1.00 | 20.29 | AAAA |
| ATOM | 1721 | OD1 | ASN A 217 | 22.089 | 19.888 | 60.499 | 1.00 | 18.03 | AAAA |
| ATOM | 1722 | ND2 | ASN A 217 | 24.274 | 19.790 | 60.004 | 1.00 | 19.95 | AAAA |
| ATOM | 1723 | C | ASN A 217 | 22.216 | 19.346 | 63.605 | 1.00 | 21.64 | AAAA |
| ATOM | 1724 | O | ASN A 217 | 21.263 | 18.576 | 63.757 | 1.00 | 20.34 | AAAA |
| ATOM | 1725 | N | LEU A 218 | 22.165 | 20.647 | 63.873 | 1.00 | 22.22 | AAAA |
| ATOM | 1726 | CA | LEU A 218 | 20.960 | 21.282 | 64.388 | 1.00 | 22.03 | AAAA |
| ATOM | 1727 | CB | LEU A 218 | 21.195 | 21.711 | 65.840 | 1.00 | 20.97 | AAAA |
| ATOM | 1728 | CG | LEU A 218 | 20.051 | 21.838 | 66.841 | 1.00 | 20.94 | AAAA |
| ATOM | 1729 | CD1 | LEU A 218 | 20.513 | 22.744 | 67.936 | 1.00 | 20.31 | AAAA |
| ATOM | 1730 | CD2 | LEU A 218 | 18.818 | 22.412 | 66.227 | 1.00 | 21.27 | AAAA |
| ATOM | 1731 | C | LEU A 218 | 20.669 | 22.513 | 63.547 | 1.00 | 22.70 | AAAA |
| ATOM | 1732 | O | LEU A 218 | 21.451 | 23.454 | 63.557 | 1.00 | 22.64 | AAAA |
| ATOM | 1733 | N | ASN A 219 | 19.564 | 22.491 | 62.808 | 1.00 | 24.00 | AAAA |
| ATOM | 1734 | CA | ASN A 219 | 19.166 | 23.626 | 61.990 | 1.00 | 25.33 | AAAA |
| ATOM | 1735 | CB | ASN A 219 | 18.656 | 23.190 | 60.614 | 1.00 | 26.94 | AAAA |
| ATOM | 1736 | CG | ASN A 219 | 19.737 | 22.601 | 59.749 | 1.00 | 26.68 | AAAA |
| ATOM | 1737 | OD1 | ASN A 219 | 20.812 | 23.169 | 59.626 | 1.00 | 28.06 | AAAA |
| ATOM | 1738 | ND2 | ASN A 219 | 19.446 | 21.471 | 59.117 | 1.00 | 26.26 | AAAA |
| ATOM | 1739 | C | ASN A 219 | 18.046 | 24.345 | 62.710 | 1.00 | 25.69 | AAAA |
| ATOM | 1740 | O | ASN A 219 | 17.118 | 23.706 | 63.210 | 1.00 | 27.51 | AAAA |
| ATOM | 1741 | N | ILE A 220 | 18.122 | 25.667 | 62.753 | 1.00 | 25.05 | AAAA |
| ATOM | 1742 | CA | ILE A 220 | 17.107 | 26.457 | 63.428 | 1.00 | 25.87 | AAAA |
| ATOM | 1743 | CB | ILE A 220 | 17.733 | 27.331 | 64.557 | 1.00 | 25.04 | AAAA |
| ATOM | 1744 | CG2 | ILE A 220 | 16.654 | 28.152 | 65.227 | 1.00 | 25.24 | AAAA |
| ATOM | 1745 | CG1 | ILE A 220 | 18.460 | 26.447 | 65.584 | 1.00 | 24.07 | AAAA |
| ATOM | 1746 | CD1 | ILE A 220 | 17.557 | 25.502 | 66.378 | 1.00 | 22.28 | AAAA |
| ATOM | 1747 | C | ILE A 220 | 16.430 | 27.370 | 62.414 | 1.00 | 26.20 | AAAA |
| ATOM | 1748 | O | ILE A 220 | 16.801 | 28.534 | 62.265 | 1.00 | 25.35 | AAAA |
| ATOM | 1749 | N | PRO A 221 | 15.421 | 26.850 | 61.704 | 1.00 | 26.70 | AAAA |
| ATOM | 1750 | CD | PRO A 221 | 14.840 | 25.501 | 61.778 | 1.00 | 27.17 | AAAA |
| ATOM | 1751 | CA | PRO A 221 | 14.706 | 27.640 | 60.703 | 1.00 | 27.67 | AAAA |
| ATOM | 1752 | CB | PRO A 221 | 13.771 | 26.613 | 60.064 | 1.00 | 26.81 | AAAA |
| ATOM | 1753 | CG | PRO A 221 | 14.473 | 25.293 | 60.346 | 1.00 | 27.36 | AAAA |
| ATOM | 1754 | C | PRO A 221 | 13.944 | 28.763 | 61.390 | 1.00 | 28.61 | AAAA |
| ATOM | 1755 | O | PRO A 221 | 13.218 | 28.515 | 62.363 | 1.00 | 29.91 | AAAA |
| ATOM | 1756 | N | LEU A 222 | 14.100 | 29.990 | 60.900 | 1.00 | 28.15 | AAAA |
| ATOM | 1757 | CA | LEU A 222 | 13.408 | 31.117 | 61.511 | 1.00 | 28.48 | AAAA |
| ATOM | 1758 | CB | LEU A 222 | 14.431 | 32.041 | 62.191 | 1.00 | 28.69 | AAAA |
| ATOM | 1759 | CG | LEU A 222 | 15.187 | 31.394 | 63.371 | 1.00 | 28.67 | AAAA |
| ATOM | 1760 | CD1 | LEU A 222 | 16.304 | 32.300 | 63.837 | 1.00 | 28.62 | AAAA |
| ATOM | 1761 | CD2 | LEU A 222 | 14.231 | 31.106 | 64.527 | 1.00 | 27.65 | AAAA |
| ATOM | 1762 | C | LEU A 222 | 12.726 | 31.882 | 60.518 | 1.00 | 28.44 | AAAA |
| ATOM | 1763 | O | LEU A 222 | 12.118 | 31.958 | 59.325 | 1.00 | 27.90 | AAAA |
| ATOM | 1764 | N | PRO A 223 | 11.113 | 32.441 | 61.009 | 1.00 | 28.79 | AAAA |
| ATOM | 1765 | CD | PRO A 223 | 10.966 | 32.357 | 62.410 | 1.00 | 29.20 | AAAA |
| ATOM | 1766 | CA | PRO A 223 | 10.437 | 33.202 | 60.227 | 1.00 | 29.36 | AAAA |
| ATOM | 1767 | CB | PRO A 223 | 9.256 | 33.287 | 61.183 | 1.00 | 28.98 | AAAA |
| ATOM | 1768 | CG | PRO A 223 | 9.965 | 33.502 | 62.485 | 1.00 | 28.68 | AAAA |
| ATOM | 1769 | C | PRO A 223 | 10.890 | 34.585 | 59.753 | 1.00 | 30.15 | AAAA |
| ATOM | 1770 | O | PRO A 223 | 11.864 | 35.152 | 60.253 | 1.00 | 30.18 | AAAA |
| ATOM | 1771 | N | LYS A 224 | 10.150 | 35.112 | 58.781 | 1.00 | 30.50 | AAAA |
| ATOM | 1772 | CA | LYS A 224 | 10.398 | 36.422 | 58.213 | 1.00 | 29.92 | AAAA |
| ATOM | 1773 | CB | LYS A 224 | 9.491 | 36.661 | 57.008 | 1.00 | 30.57 | AAAA |
| ATOM | 1774 | CG | LYS A 224 | 9.588 | 35.676 | 55.893 | 1.00 | 30.06 | AAAA |
| ATOM | 1775 | CD | LYS A 224 | 8.640 | 36.087 | 54.798 | 1.00 | 30.91 | AAAA |
| ATOM | 1776 | CE | LYS A 224 | 8.575 | 35.051 | 53.705 | 1.00 | 32.15 | AAAA |
| ATOM | 1777 | NZ | LYS A 224 | 7.628 | 35.476 | 52.648 | 1.00 | 32.75 | AAAA |
| ATOM | 1778 | C | LYS A 224 | 10.050 | 37.468 | 59.260 | 1.00 | 29.75 | AAAA |
| ATOM | 1779 | O | LYS A 224 | 9.308 | 37.193 | 60.196 | 1.00 | 29.84 | AAAA |
| ATOM | 1780 | N | GLY A 225 | 10.555 | 38.678 | 59.079 | 1.00 | 29.39 | AAAA |
| ATOM | 1781 | CA | GLY A 225 | 10.261 | 39.730 | 60.031 | 1.00 | 29.87 | AAAA |
| ATOM | 1782 | C | GLY A 225 | 10.809 | 39.447 | 61.415 | 1.00 | 29.85 | AAAA |

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Figure 19-28

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|------|
| ATOM | 1783 | O | GLY A 225 | 10.371 | 40.051 | 62.392 | 1.00 | 29.85 | AAAA |
| ATOM | 1784 | N | LEU A 226 | 11.775 | 38.536 | 61.499 | 1.00 | 29.50 | AAAA |
| ATOM | 1785 | CA | LEU A 226 | 12.374 | 38.175 | 62.778 | 1.00 | 29.80 | AAAA |
| ATOM | 1786 | CB | LEU A 226 | 13.513 | 37.170 | 62.570 | 1.00 | 28.81 | AAAA |
| ATOM | 1787 | CG | LEU A 226 | 14.097 | 36.514 | 63.820 | 1.00 | 27.29 | AAAA |
| ATOM | 1788 | CD1 | LEU A 226 | 13.132 | 35.452 | 64.275 | 1.00 | 26.06 | AAAA |
| ATOM | 1789 | CD2 | LEU A 226 | 15.455 | 35.888 | 63.538 | 1.00 | 27.03 | AAAA |
| ATOM | 1790 | C | LEU A 226 | 12.936 | 39.428 | 63.448 | 1.00 | 30.68 | AAAA |
| ATOM | 1791 | O | LEU A 226 | 13.636 | 40.217 | 62.804 | 1.00 | 30.57 | AAAA |
| ATOM | 1792 | N | ASN A 227 | 12.624 | 39.617 | 64.729 | 1.00 | 31.46 | AAAA |
| ATOM | 1793 | CA | ASN A 227 | 13.139 | 40.769 | 65.469 | 1.00 | 32.06 | AAAA |
| ATOM | 1794 | CB | ASN A 227 | 12.012 | 41.507 | 66.217 | 1.00 | 31.74 | AAAA |
| ATOM | 1795 | CG | ASN A 227 | 11.291 | 40.630 | 67.234 | 1.00 | 32.07 | AAAA |
| ATOM | 1796 | OD1 | ASN A 227 | 11.914 | 40.017 | 68.104 | 1.00 | 31.61 | AAAA |
| ATOM | 1797 | ND2 | ASN A 227 | 9.962 | 40.592 | 67.141 | 1.00 | 31.59 | AAAA |
| ATOM | 1798 | C | ASN A 227 | 14.225 | 40.334 | 66.444 | 1.00 | 32.45 | AAAA |
| ATOM | 1799 | O | ASN A 227 | 14.413 | 39.140 | 66.688 | 1.00 | 32.78 | AAAA |
| ATOM | 1800 | N | ASP A 228 | 14.943 | 41.297 | 67.002 | 1.00 | 33.32 | AAAA |
| ATOM | 1801 | CA | ASP A 228 | 16.017 | 40.976 | 67.928 | 1.00 | 34.75 | AAAA |
| ATOM | 1802 | CB | ASP A 228 | 16.508 | 42.233 | 68.654 | 1.00 | 36.77 | AAAA |
| ATOM | 1803 | CG | ASP A 228 | 17.154 | 43.238 | 67.714 | 1.00 | 37.28 | AAAA |
| ATOM | 1804 | OD1 | ASP A 228 | 17.662 | 42.816 | 66.652 | 1.00 | 37.78 | AAAA |
| ATOM | 1805 | OD2 | ASP A 228 | 17.180 | 44.443 | 68.054 | 1.00 | 37.21 | AAAA |
| ATOM | 1806 | C | ASP A 228 | 15.707 | 39.892 | 68.964 | 1.00 | 34.93 | AAAA |
| ATOM | 1807 | O | ASP A 228 | 16.448 | 38.919 | 69.056 | 1.00 | 36.92 | AAAA |
| ATOM | 1808 | N | ASN A 229 | 14.635 | 40.054 | 69.741 | 1.00 | 33.90 | AAAA |
| ATOM | 1809 | CA | ASN A 229 | 14.268 | 39.079 | 70.775 | 1.00 | 33.01 | AAAA |
| ATOM | 1810 | CB | ASN A 229 | 12.965 | 39.481 | 71.455 | 1.00 | 33.79 | AAAA |
| ATOM | 1811 | CG | ASN A 229 | 13.131 | 40.663 | 72.369 | 1.00 | 34.04 | AAAA |
| ATOM | 1812 | OD1 | ASN A 229 | 13.783 | 40.564 | 73.405 | 1.00 | 34.25 | AAAA |
| ATOM | 1813 | ND2 | ASN A 229 | 12.550 | 41.797 | 71.988 | 1.00 | 34.05 | AAAA |
| ATOM | 1814 | C | ASN A 229 | 14.114 | 37.656 | 70.276 | 1.00 | 32.98 | AAAA |
| ATOM | 1815 | O | ASN A 229 | 14.529 | 36.697 | 70.944 | 1.00 | 32.77 | AAAA |
| ATOM | 1816 | N | GLU A 230 | 13.496 | 37.523 | 69.108 | 1.00 | 32.02 | AAAA |
| ATOM | 1817 | CA | GLU A 230 | 13.277 | 36.227 | 68.516 | 1.00 | 30.72 | AAAA |
| ATOM | 1818 | CB | GLU A 230 | 12.399 | 36.375 | 67.272 | 1.00 | 31.38 | AAAA |
| ATOM | 1819 | CG | GLU A 230 | 11.006 | 36.896 | 67.583 | 1.00 | 31.02 | AAAA |
| ATOM | 1820 | CD | GLU A 230 | 10.175 | 37.187 | 66.350 | 1.00 | 31.52 | AAAA |
| ATOM | 1821 | OE1 | GLU A 230 | 10.644 | 37.970 | 65.497 | 1.00 | 31.89 | AAAA |
| ATOM | 1822 | OE2 | GLU A 230 | 9.047 | 36.655 | 66.241 | 1.00 | 31.04 | AAAA |
| ATOM | 1823 | C | GLU A 230 | 14.628 | 35.622 | 68.180 | 1.00 | 30.79 | AAAA |
| ATOM | 1824 | O | GLU A 230 | 14.905 | 34.465 | 68.512 | 1.00 | 31.05 | AAAA |
| ATOM | 1825 | N | PHE A 231 | 15.490 | 36.412 | 67.553 | 1.00 | 30.05 | AAAA |
| ATOM | 1826 | CA | PHE A 231 | 16.811 | 35.920 | 67.191 | 1.00 | 28.94 | AAAA |
| ATOM | 1827 | CB | PHE A 231 | 17.632 | 37.015 | 66.528 | 1.00 | 29.33 | AAAA |
| ATOM | 1828 | CG | PHE A 231 | 18.949 | 36.537 | 65.972 | 1.00 | 28.79 | AAAA |
| ATOM | 1829 | CD1 | PHE A 231 | 18.982 | 35.585 | 64.957 | 1.00 | 28.93 | AAAA |
| ATOM | 1830 | CD2 | PHE A 231 | 20.152 | 37.067 | 66.436 | 1.00 | 28.55 | AAAA |
| ATOM | 1831 | CE1 | PHE A 231 | 20.195 | 35.160 | 64.397 | 1.00 | 28.32 | AAAA |
| ATOM | 1832 | CE2 | PHE A 231 | 21.376 | 36.657 | 65.888 | 1.00 | 28.97 | AAAA |
| ATOM | 1833 | CZ | PHE A 231 | 21.397 | 35.695 | 64.860 | 1.00 | 28.81 | AAAA |
| ATOM | 1834 | C | PHE A 231 | 17.559 | 35.443 | 68.413 | 1.00 | 28.25 | AAAA |
| ATOM | 1835 | O | PHE A 231 | 17.999 | 34.302 | 68.485 | 1.00 | 27.97 | AAAA |
| ATOM | 1836 | N | LEU A 232 | 17.691 | 36.329 | 69.384 | 1.00 | 27.93 | AAAA |
| ATOM | 1837 | CA | LEU A 232 | 18.425 | 36.003 | 70.590 | 1.00 | 27.93 | AAAA |
| ATOM | 1838 | CB | LEU A 232 | 18.521 | 37.234 | 71.484 | 1.00 | 28.16 | AAAA |
| ATOM | 1839 | CG | LEU A 232 | 19.220 | 38.379 | 70.747 | 1.00 | 27.96 | AAAA |
| ATOM | 1840 | CD1 | LEU A 232 | 19.203 | 39.629 | 71.587 | 1.00 | 27.57 | AAAA |
| ATOM | 1841 | CD2 | LEU A 232 | 20.639 | 37.955 | 70.387 | 1.00 | 27.76 | AAAA |
| ATOM | 1842 | C | LEU A 232 | 17.815 | 34.851 | 71.340 | 1.00 | 27.95 | AAAA |
| ATOM | 1843 | O | LEU A 232 | 18.526 | 34.061 | 71.941 | 1.00 | 27.92 | AAAA |
| ATOM | 1844 | N | PHE A 233 | 16.495 | 34.758 | 71.298 | 1.00 | 28.81 | AAAA |
| ATOM | 1845 | CA | PHE A 233 | 15.786 | 33.685 | 71.972 | 1.00 | 30.27 | AAAA |
| ATOM | 1846 | CB | PHE A 233 | 14.278 | 33.837 | 71.745 | 1.00 | 31.51 | AAAA |
| ATOM | 1847 | CG | PHE A 233 | 13.465 | 32.710 | 72.308 | 1.00 | 32.38 | AAAA |
| ATOM | 1848 | CD1 | PHE A 233 | 13.257 | 32.599 | 73.677 | 1.00 | 33.66 | AAAA |

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Figure 19-29

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1849 | CD2 | PHE | A | 233 | 12.928 | 31.741 | 71.467 | 1.00 | 33.51 | AAAA |
| ATOM | 1850 | CE1 | PHE | A | 233 | 12.518 | 31.537 | 74.201 | 1.00 | 35.10 | AAAA |
| ATOM | 1851 | CE2 | PHE | A | 233 | 12.193 | 30.677 | 71.975 | 1.00 | 34.21 | AAAA |
| ATOM | 1852 | CZ | PHE | A | 233 | 11.986 | 30.572 | 73.344 | 1.00 | 35.23 | AAAA |
| ATOM | 1853 | C | PHE | A | 233 | 16.219 | 32.301 | 71.483 | 1.00 | 30.55 | AAAA |
| ATOM | 1854 | O | PHE | A | 233 | 16.438 | 31.391 | 72.280 | 1.00 | 30.65 | AAAA |
| ATOM | 1855 | N | ALA | A | 234 | 16.317 | 32.151 | 70.165 | 1.00 | 30.21 | AAAA |
| ATOM | 1856 | CA | ALA | A | 234 | 16.698 | 30.892 | 69.549 | 1.00 | 28.97 | AAAA |
| ATOM | 1857 | CB | ALA | A | 234 | 16.398 | 30.942 | 68.065 | 1.00 | 30.40 | AAAA |
| ATOM | 1858 | C | ALA | A | 234 | 18.169 | 30.571 | 69.761 | 1.00 | 28.27 | AAAA |
| ATOM | 1859 | O | ALA | A | 234 | 18.564 | 29.401 | 69.830 | 1.00 | 26.69 | AAAA |
| ATOM | 1860 | N | LEU | A | 235 | 18.978 | 31.614 | 69.855 | 1.00 | 27.56 | AAAA |
| ATOM | 1861 | CA | LEU | A | 235 | 20.402 | 31.427 | 70.055 | 1.00 | 29.17 | AAAA |
| ATOM | 1862 | CB | LEU | A | 235 | 21.126 | 32.767 | 69.989 | 1.00 | 29.04 | AAAA |
| ATOM | 1863 | CG | LEU | A | 235 | 22.527 | 32.757 | 69.378 | 1.00 | 28.54 | AAAA |
| ATOM | 1864 | CD1 | LEU | A | 235 | 23.350 | 33.837 | 70.058 | 1.00 | 27.05 | AAAA |
| ATOM | 1865 | CD2 | LEU | A | 235 | 23.182 | 31.408 | 69.558 | 1.00 | 27.21 | AAAA |
| ATOM | 1866 | C | LEU | A | 235 | 20.637 | 30.799 | 71.429 | 1.00 | 30.99 | AAAA |
| ATOM | 1867 | O | LEU | A | 235 | 21.159 | 29.697 | 71.547 | 1.00 | 31.65 | AAAA |
| ATOM | 1868 | N | GLU | A | 236 | 20.242 | 31.514 | 72.471 | 1.00 | 31.88 | AAAA |
| ATOM | 1869 | CA | GLU | A | 236 | 20.409 | 31.042 | 73.838 | 1.00 | 32.99 | AAAA |
| ATOM | 1870 | CB | GLU | A | 236 | 19.689 | 31.990 | 74.790 | 1.00 | 34.63 | AAAA |
| ATOM | 1871 | CG | GLU | A | 236 | 19.980 | 33.449 | 74.531 | 1.00 | 36.79 | AAAA |
| ATOM | 1872 | CD | GLU | A | 236 | 19.044 | 34.360 | 75.294 | 1.00 | 38.99 | AAAA |
| ATOM | 1873 | OE1 | GLU | A | 236 | 17.803 | 34.303 | 75.070 | 1.00 | 39.03 | AAAA |
| ATOM | 1874 | OE2 | GLU | A | 236 | 19.559 | 35.132 | 76.126 | 1.00 | 41.56 | AAAA |
| ATOM | 1875 | C | GLU | A | 236 | 19.806 | 29.656 | 73.982 | 1.00 | 32.94 | AAAA |
| ATOM | 1876 | O | GLU | A | 236 | 20.379 | 28.753 | 74.595 | 1.00 | 31.76 | AAAA |
| ATOM | 1877 | N | LYS | A | 237 | 18.631 | 29.503 | 73.399 | 1.00 | 32.83 | AAAA |
| ATOM | 1878 | CA | LYS | A | 237 | 17.906 | 28.256 | 73.471 | 1.00 | 33.59 | AAAA |
| ATOM | 1879 | CB | LYS | A | 237 | 16.504 | 28.506 | 72.942 | 1.00 | 35.00 | AAAA |
| ATOM | 1880 | CG | LYS | A | 237 | 15.516 | 27.436 | 73.213 | 1.00 | 36.69 | AAAA |
| ATOM | 1881 | CD | LYS | A | 237 | 14.310 | 28.008 | 73.940 | 1.00 | 38.53 | AAAA |
| ATOM | 1882 | CE | LYS | A | 237 | 14.636 | 28.331 | 75.392 | 1.00 | 39.27 | AAAA |
| ATOM | 1883 | NZ | LYS | A | 237 | 13.398 | 28.531 | 76.204 | 1.00 | 39.42 | AAAA |
| ATOM | 1884 | C | LYS | A | 237 | 18.619 | 27.129 | 72.707 | 1.00 | 33.14 | AAAA |
| ATOM | 1885 | O | LYS | A | 237 | 18.850 | 26.051 | 73.260 | 1.00 | 33.29 | AAAA |
| ATOM | 1886 | N | SER | A | 238 | 18.985 | 27.374 | 71.452 | 1.00 | 32.13 | AAAA |
| ATOM | 1887 | CA | SER | A | 238 | 19.671 | 26.345 | 70.685 | 1.00 | 31.25 | AAAA |
| ATOM | 1888 | CB | SER | A | 238 | 19.740 | 26.717 | 69.194 | 1.00 | 30.52 | AAAA |
| ATOM | 1889 | OG | SER | A | 238 | 20.544 | 27.851 | 68.970 | 1.00 | 29.95 | AAAA |
| ATOM | 1890 | C | SER | A | 238 | 21.075 | 26.064 | 71.236 | 1.00 | 31.21 | AAAA |
| ATOM | 1891 | O | SER | A | 238 | 21.556 | 24.929 | 71.169 | 1.00 | 30.06 | AAAA |
| ATOM | 1892 | N | LEU | A | 239 | 21.740 | 27.077 | 71.782 | 1.00 | 31.71 | AAAA |
| ATOM | 1893 | CA | LEU | A | 239 | 23.070 | 26.842 | 72.351 | 1.00 | 33.47 | AAAA |
| ATOM | 1894 | CB | LEU | A | 239 | 23.698 | 28.130 | 72.900 | 1.00 | 31.25 | AAAA |
| ATOM | 1895 | CG | LEU | A | 239 | 23.988 | 29.301 | 71.977 | 1.00 | 29.80 | AAAA |
| ATOM | 1896 | CD1 | LEU | A | 239 | 24.589 | 30.414 | 72.787 | 1.00 | 29.05 | AAAA |
| ATOM | 1897 | CD2 | LEU | A | 239 | 24.919 | 28.903 | 70.872 | 1.00 | 29.36 | AAAA |
| ATOM | 1898 | C | LEU | A | 239 | 22.933 | 25.839 | 73.502 | 1.00 | 35.41 | AAAA |
| ATOM | 1899 | O | LEU | A | 239 | 23.812 | 25.012 | 73.735 | 1.00 | 36.25 | AAAA |
| ATOM | 1900 | N | GLU | A | 240 | 21.816 | 25.906 | 74.213 | 1.00 | 37.34 | AAAA |
| ATOM | 1901 | CA | GLU | A | 240 | 21.594 | 25.005 | 75.331 | 1.00 | 39.39 | AAAA |
| ATOM | 1902 | CB | GLU | A | 240 | 20.281 | 25.361 | 76.017 | 1.00 | 41.90 | AAAA |
| ATOM | 1903 | CG | GLU | A | 240 | 20.040 | 24.610 | 77.308 | 1.00 | 45.52 | AAAA |
| ATOM | 1904 | CD | GLU | A | 240 | 19.665 | 25.552 | 78.432 | 1.00 | 47.80 | AAAA |
| ATOM | 1905 | OE1 | GLU | A | 240 | 18.670 | 26.295 | 78.274 | 1.00 | 49.70 | AAAA |
| ATOM | 1906 | OE2 | GLU | A | 240 | 20.364 | 25.559 | 79.469 | 1.00 | 48.04 | AAAA |
| ATOM | 1907 | C | GLU | A | 240 | 21.583 | 23.555 | 74.875 | 1.00 | 38.80 | AAAA |
| ATOM | 1908 | O | GLU | A | 240 | 22.224 | 22.700 | 75.478 | 1.00 | 37.85 | AAAA |
| ATOM | 1909 | N | ILE | A | 241 | 20.847 | 23.293 | 73.804 | 1.00 | 39.66 | AAAA |
| ATOM | 1910 | CA | ILE | A | 241 | 20.751 | 21.955 | 73.223 | 1.00 | 40.81 | AAAA |
| ATOM | 1911 | CB | ILE | A | 241 | 19.912 | 21.994 | 71.917 | 1.00 | 41.10 | AAAA |
| ATOM | 1912 | CG2 | ILE | A | 241 | 19.850 | 20.621 | 71.287 | 1.00 | 40.88 | AAAA |
| ATOM | 1913 | CG1 | ILE | A | 241 | 18.502 | 22.514 | 72.220 | 1.00 | 41.45 | AAAA |
| ATOM | 1914 | CD1 | ILE | A | 241 | 17.641 | 22.745 | 70.992 | 1.00 | 41.14 | AAAA |

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Figure 19-30

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1915 | C | ILE | A | 241 | 22.159 | 21.424 | 72.893 | 1.00 | 41.66 | AAAA |
| ATOM | 1916 | O | ILE | A | 241 | 22.445 | 20.229 | 73.045 | 1.00 | 42.10 | AAAA |
| ATOM | 1917 | N | VAL | A | 242 | 23.026 | 22.324 | 72.432 | 1.00 | 41.42 | AAAA |
| ATOM | 1918 | CA | VAL | A | 242 | 24.394 | 21.977 | 72.076 | 1.00 | 41.23 | AAAA |
| ATOM | 1919 | CB | VAL | A | 242 | 25.089 | 23.146 | 71.351 | 1.00 | 40.40 | AAAA |
| ATOM | 1920 | CG1 | VAL | A | 242 | 26.556 | 22.850 | 71.171 | 1.00 | 39.25 | AAAA |
| ATOM | 1921 | CG2 | VAL | A | 242 | 24.438 | 23.384 | 70.004 | 1.00 | 39.79 | AAAA |
| ATOM | 1922 | C | VAL | A | 242 | 25.228 | 21.604 | 73.298 | 1.00 | 42.67 | AAAA |
| ATOM | 1923 | O | VAL | A | 242 | 25.882 | 20.562 | 73.316 | 1.00 | 41.83 | AAAA |
| ATOM | 1924 | N | LYS | A | 243 | 25.198 | 22.456 | 74.318 | 1.00 | 44.41 | AAAA |
| ATOM | 1925 | CA | LYS | A | 243 | 25.972 | 22.215 | 75.523 | 1.00 | 46.51 | AAAA |
| ATOM | 1926 | CB | LYS | A | 243 | 25.797 | 23.363 | 76.522 | 1.00 | 47.29 | AAAA |
| ATOM | 1927 | CG | LYS | A | 243 | 26.820 | 23.312 | 77.664 | 1.00 | 48.40 | AAAA |
| ATOM | 1928 | CD | LYS | A | 243 | 26.479 | 24.248 | 78.823 | 1.00 | 48.88 | AAAA |
| ATOM | 1929 | CE | LYS | A | 243 | 26.355 | 25.691 | 78.380 | 1.00 | 49.62 | AAAA |
| ATOM | 1930 | NZ | LYS | A | 243 | 25.926 | 26.576 | 79.505 | 1.00 | 50.11 | AAAA |
| ATOM | 1931 | C | LYS | A | 243 | 25.639 | 20.891 | 76.209 | 1.00 | 47.59 | AAAA |
| ATOM | 1932 | O | LYS | A | 243 | 26.537 | 20.216 | 76.711 | 1.00 | 48.17 | AAAA |
| ATOM | 1933 | N | GLU | A | 244 | 24.362 | 20.517 | 76.237 | 1.00 | 48.86 | AAAA |
| ATOM | 1934 | CA | GLU | A | 244 | 23.957 | 19.262 | 76.877 | 1.00 | 50.82 | AAAA |
| ATOM | 1935 | CB | GLU | A | 244 | 22.432 | 19.208 | 77.103 | 1.00 | 52.08 | AAAA |
| ATOM | 1936 | CG | GLU | A | 244 | 21.818 | 20.405 | 77.829 | 1.00 | 53.82 | AAAA |
| ATOM | 1937 | CD | GLU | A | 244 | 20.359 | 20.174 | 78.230 | 1.00 | 54.49 | AAAA |
| ATOM | 1938 | OE1 | GLU | A | 244 | 19.666 | 21.158 | 78.595 | 1.00 | 55.15 | AAAA |
| ATOM | 1939 | OE2 | GLU | A | 244 | 19.912 | 19.006 | 78.200 | 1.00 | 54.98 | AAAA |
| ATOM | 1940 | C | GLU | A | 244 | 24.338 | 18.046 | 76.033 | 1.00 | 51.06 | AAAA |
| ATOM | 1941 | O | GLU | A | 244 | 24.206 | 16.905 | 76.477 | 1.00 | 51.68 | AAAA |
| ATOM | 1942 | N | VAL | A | 245 | 24.810 | 18.292 | 74.820 | 1.00 | 51.12 | AAAA |
| ATOM | 1943 | CA | VAL | A | 245 | 25.149 | 17.212 | 73.904 | 1.00 | 50.08 | AAAA |
| ATOM | 1944 | CB | VAL | A | 245 | 24.217 | 17.263 | 72.677 | 1.00 | 50.22 | AAAA |
| ATOM | 1945 | CG1 | VAL | A | 245 | 24.615 | 16.217 | 71.651 | 1.00 | 51.07 | AAAA |
| ATOM | 1946 | CG2 | VAL | A | 245 | 22.794 | 17.049 | 73.118 | 1.00 | 50.79 | AAAA |
| ATOM | 1947 | C | VAL | A | 245 | 26.578 | 17.254 | 73.397 | 1.00 | 49.43 | AAAA |
| ATOM | 1948 | O | VAL | A | 245 | 27.101 | 16.250 | 72.917 | 1.00 | 48.65 | AAAA |
| ATOM | 1949 | N | PHE | A | 246 | 27.220 | 18.408 | 73.522 | 1.00 | 48.65 | AAAA |
| ATOM | 1950 | CA | PHE | A | 246 | 28.556 | 18.552 | 72.982 | 1.00 | 47.97 | AAAA |
| ATOM | 1951 | CB | PHE | A | 246 | 28.420 | 19.212 | 71.607 | 1.00 | 46.45 | AAAA |
| ATOM | 1952 | CG | PHE | A | 246 | 29.553 | 18.932 | 70.671 | 1.00 | 45.35 | AAAA |
| ATOM | 1953 | CD1 | PHE | A | 246 | 29.841 | 17.629 | 70.280 | 1.00 | 44.13 | AAAA |
| ATOM | 1954 | CD2 | PHE | A | 246 | 30.291 | 19.972 | 70.124 | 1.00 | 44.40 | AAAA |
| ATOM | 1955 | CE1 | PHE | A | 246 | 30.840 | 17.370 | 69.356 | 1.00 | 43.95 | AAAA |
| ATOM | 1956 | CE2 | PHE | A | 246 | 31.292 | 19.721 | 69.197 | 1.00 | 43.47 | AAAA |
| ATOM | 1957 | CZ | PHE | A | 246 | 31.566 | 18.422 | 68.811 | 1.00 | 44.05 | AAAA |
| ATOM | 1958 | C | PHE | A | 246 | 29.481 | 19.383 | 73.860 | 1.00 | 48.60 | AAAA |
| ATOM | 1959 | O | PHE | A | 246 | 29.132 | 20.501 | 74.239 | 1.00 | 49.59 | AAAA |
| ATOM | 1960 | N | GLU | A | 247 | 30.647 | 18.834 | 74.198 | 1.00 | 48.69 | AAAA |
| ATOM | 1961 | CA | GLU | A | 247 | 31.644 | 19.578 | 74.977 | 1.00 | 49.45 | AAAA |
| ATOM | 1962 | CB | GLU | A | 247 | 32.174 | 18.768 | 76.178 | 1.00 | 51.91 | AAAA |
| ATOM | 1963 | CG | GLU | A | 247 | 31.257 | 18.659 | 77.398 | 1.00 | 54.39 | AAAA |
| ATOM | 1964 | CD | GLU | A | 247 | 29.986 | 17.845 | 77.146 | 1.00 | 57.34 | AAAA |
| ATOM | 1965 | OE1 | GLU | A | 247 | 29.100 | 18.315 | 76.393 | 1.00 | 58.48 | AAAA |
| ATOM | 1966 | OE2 | GLU | A | 247 | 29.877 | 16.725 | 77.702 | 1.00 | 57.95 | AAAA |
| ATOM | 1967 | C | GLU | A | 247 | 32.807 | 19.903 | 74.024 | 1.00 | 47.39 | AAAA |
| ATOM | 1968 | O | GLU | A | 247 | 33.742 | 19.119 | 73.872 | 1.00 | 46.65 | AAAA |
| ATOM | 1969 | N | PRO | A | 248 | 32.748 | 21.070 | 73.371 | 1.00 | 46.25 | AAAA |
| ATOM | 1970 | CD | PRO | A | 248 | 31.651 | 22.033 | 73.543 | 1.00 | 46.49 | AAAA |
| ATOM | 1971 | CA | PRO | A | 248 | 33.710 | 21.614 | 72.411 | 1.00 | 45.44 | AAAA |
| ATOM | 1972 | CB | PRO | A | 248 | 33.063 | 22.948 | 72.017 | 1.00 | 45.57 | AAAA |
| ATOM | 1973 | CG | PRO | A | 248 | 31.604 | 22.661 | 72.178 | 1.00 | 46.28 | AAAA |
| ATOM | 1974 | C | PRO | A | 248 | 35.155 | 21.814 | 72.880 | 1.00 | 44.29 | AAAA |
| ATOM | 1975 | O | PRO | A | 248 | 35.401 | 22.370 | 73.947 | 1.00 | 44.57 | AAAA |
| ATOM | 1976 | N | GLU | A | 249 | 36.100 | 21.364 | 72.059 | 1.00 | 42.21 | AAAA |
| ATOM | 1977 | CA | GLU | A | 249 | 37.522 | 21.526 | 72.340 | 1.00 | 39.87 | AAAA |
| ATOM | 1978 | CB | GLU | A | 249 | 38.344 | 20.460 | 71.625 | 1.00 | 39.58 | AAAA |
| ATOM | 1979 | CG | GLU | A | 249 | 37.960 | 19.030 | 71.957 | 1.00 | 41.32 | AAAA |
| ATOM | 1980 | CD | GLU | A | 249 | 38.825 | 18.007 | 71.241 | 1.00 | 40.96 | AAAA |

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Figure 19-31

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 1981 | OE1 | GLU | A | 249 | 38.871 | 18.017 | 69.996 | 1.00 | 41.55 | AAAA |
| ATOM | 1982 | OE2 | GLU | A | 249 | 39.462 | 17.187 | 71.926 | 1.00 | 42.49 | AAAA |
| ATOM | 1983 | C | GLU | A | 249 | 37.840 | 22.873 | 71.718 | 1.00 | 38.81 | AAAA |
| ATOM | 1984 | O | GLU | A | 249 | 38.715 | 23.617 | 72.181 | 1.00 | 38.27 | AAAA |
| ATOM | 1985 | N | VAL | A | 250 | 37.109 | 23.160 | 70.644 | 1.00 | 36.60 | AAAA |
| ATOM | 1986 | CA | VAL | A | 250 | 37.242 | 24.402 | 69.890 | 1.00 | 34.20 | AAAA |
| ATOM | 1987 | CB | VAL | A | 250 | 38.379 | 24.321 | 68.862 | 1.00 | 33.73 | AAAA |
| ATOM | 1988 | CG1 | VAL | A | 250 | 38.085 | 23.209 | 67.864 | 1.00 | 33.26 | AAAA |
| ATOM | 1989 | CG2 | VAL | A | 250 | 38.546 | 25.678 | 68.153 | 1.00 | 33.75 | AAAA |
| ATOM | 1990 | C | VAL | A | 250 | 35.945 | 24.617 | 69.130 | 1.00 | 31.98 | AAAA |
| ATOM | 1991 | O | VAL | A | 250 | 35.205 | 23.658 | 68.904 | 1.00 | 32.36 | AAAA |
| ATOM | 1992 | N | TYR | A | 251 | 35.657 | 25.863 | 68.760 | 1.00 | 28.65 | AAAA |
| ATOM | 1993 | CA | TYR | A | 251 | 34.449 | 26.150 | 67.991 | 1.00 | 26.49 | AAAA |
| ATOM | 1994 | CB | TYR | A | 251 | 33.241 | 26.442 | 68.906 | 1.00 | 24.32 | AAAA |
| ATOM | 1995 | CG | TYR | A | 251 | 33.193 | 27.853 | 69.465 | 1.00 | 22.96 | AAAA |
| ATOM | 1996 | CD1 | TYR | A | 251 | 32.771 | 28.931 | 68.668 | 1.00 | 22.21 | AAAA |
| ATOM | 1997 | CE1 | TYR | A | 251 | 32.791 | 30.234 | 69.151 | 1.00 | 21.29 | AAAA |
| ATOM | 1998 | CD2 | TYR | A | 251 | 33.628 | 28.124 | 70.771 | 1.00 | 21.47 | AAAA |
| ATOM | 1999 | CE2 | TYR | A | 251 | 33.651 | 29.425 | 71.265 | 1.00 | 20.80 | AAAA |
| ATOM | 2000 | CZ | TYR | A | 251 | 33.237 | 30.475 | 70.449 | 1.00 | 20.77 | AAAA |
| ATOM | 2001 | OH | TYR | A | 251 | 33.309 | 31.768 | 70.913 | 1.00 | 21.41 | AAAA |
| ATOM | 2002 | C | TYR | A | 251 | 34.691 | 27.345 | 67.092 | 1.00 | 24.59 | AAAA |
| ATOM | 2003 | O | TYR | A | 251 | 35.504 | 28.216 | 67.410 | 1.00 | 25.87 | AAAA |
| ATOM | 2004 | N | LEU | A | 252 | 33.984 | 27.374 | 65.970 | 1.00 | 22.49 | AAAA |
| ATOM | 2005 | CA | LEU | A | 252 | 34.082 | 28.482 | 65.045 | 1.00 | 20.96 | AAAA |
| ATOM | 2006 | CB | LEU | A | 252 | 34.523 | 28.018 | 63.657 | 1.00 | 21.31 | AAAA |
| ATOM | 2007 | CG | LEU | A | 252 | 35.940 | 27.472 | 63.556 | 1.00 | 21.03 | AAAA |
| ATOM | 2008 | CD1 | LEU | A | 252 | 35.947 | 26.028 | 63.977 | 1.00 | 22.16 | AAAA |
| ATOM | 2009 | CD2 | LEU | A | 252 | 36.440 | 27.594 | 62.143 | 1.00 | 22.13 | AAAA |
| ATOM | 2010 | C | LEU | A | 252 | 32.731 | 29.159 | 64.959 | 1.00 | 19.60 | AAAA |
| ATOM | 2011 | O | LEU | A | 252 | 31.689 | 28.523 | 65.070 | 1.00 | 19.95 | AAAA |
| ATOM | 2012 | N | LEU | A | 253 | 32.748 | 30.461 | 64.756 | 1.00 | 17.95 | AAAA |
| ATOM | 2013 | CA | LEU | A | 253 | 31.521 | 31.222 | 64.675 | 1.00 | 17.33 | AAAA |
| ATOM | 2014 | CB | LEU | A | 253 | 31.441 | 32.142 | 65.900 | 1.00 | 16.31 | AAAA |
| ATOM | 2015 | CG | LEU | A | 253 | 30.266 | 33.070 | 66.153 | 1.00 | 15.81 | AAAA |
| ATOM | 2016 | CD1 | LEU | A | 253 | 28.990 | 32.267 | 66.377 | 1.00 | 14.74 | AAAA |
| ATOM | 2017 | CD2 | LEU | A | 253 | 30.602 | 33.925 | 67.368 | 1.00 | 15.83 | AAAA |
| ATOM | 2018 | C | LEU | A | 253 | 31.564 | 32.035 | 63.386 | 1.00 | 16.60 | AAAA |
| ATOM | 2019 | O | LEU | A | 253 | 32.548 | 32.722 | 63.132 | 1.00 | 16.40 | AAAA |
| ATOM | 2020 | N | GLN | A | 254 | 30.526 | 31.936 | 62.557 | 1.00 | 15.88 | AAAA |
| ATOM | 2021 | CA | GLN | A | 254 | 30.507 | 32.716 | 61.328 | 1.00 | 16.27 | AAAA |
| ATOM | 2022 | CB | GLN | A | 254 | 30.045 | 31.881 | 60.121 | 1.00 | 15.88 | AAAA |
| ATOM | 2023 | CG | GLN | A | 254 | 28.587 | 32.048 | 59.734 | 1.00 | 18.52 | AAAA |
| ATOM | 2024 | CD | GLN | A | 254 | 28.380 | 32.935 | 58.519 | 1.00 | 17.54 | AAAA |
| ATOM | 2025 | OE1 | GLN | A | 254 | 28.714 | 32.572 | 57.391 | 1.00 | 15.89 | AAAA |
| ATOM | 2026 | NE2 | GLN | A | 254 | 27.828 | 34.103 | 58.750 | 1.00 | 18.49 | AAAA |
| ATOM | 2027 | C | GLN | A | 254 | 29.527 | 33.825 | 61.650 | 1.00 | 16.91 | AAAA |
| ATOM | 2028 | O | GLN | A | 254 | 28.450 | 33.571 | 62.198 | 1.00 | 17.41 | AAAA |
| ATOM | 2029 | N | LEU | A | 255 | 29.911 | 35.053 | 61.319 | 1.00 | 16.68 | AAAA |
| ATOM | 2030 | CA | LEU | A | 255 | 29.102 | 36.215 | 61.619 | 1.00 | 16.42 | AAAA |
| ATOM | 2031 | CB | LEU | A | 255 | 29.861 | 37.080 | 62.616 | 1.00 | 14.93 | AAAA |
| ATOM | 2032 | CG | LEU | A | 255 | 30.269 | 36.301 | 63.860 | 1.00 | 13.90 | AAAA |
| ATOM | 2033 | CD1 | LEU | A | 255 | 31.494 | 36.924 | 64.515 | 1.00 | 12.24 | AAAA |
| ATOM | 2034 | CD2 | LEU | A | 255 | 29.083 | 36.202 | 64.774 | 1.00 | 12.80 | AAAA |
| ATOM | 2035 | C | LEU | A | 255 | 28.699 | 37.048 | 60.404 | 1.00 | 18.32 | AAAA |
| ATOM | 2036 | O | LEU | A | 255 | 29.170 | 38.177 | 60.216 | 1.00 | 17.59 | AAAA |
| ATOM | 2037 | N | GLY | A | 256 | 27.813 | 36.482 | 59.588 | 1.00 | 19.75 | AAAA |
| ATOM | 2038 | CA | GLY | A | 256 | 27.322 | 37.188 | 58.422 | 1.00 | 20.77 | AAAA |
| ATOM | 2039 | C | GLY | A | 256 | 26.422 | 38.302 | 58.927 | 1.00 | 21.73 | AAAA |
| ATOM | 2040 | O | GLY | A | 256 | 25.642 | 38.096 | 59.857 | 1.00 | 21.38 | AAAA |
| ATOM | 2041 | N | THR | A | 257 | 26.528 | 39.485 | 58.325 | 1.00 | 22.82 | AAAA |
| ATOM | 2042 | CA | THR | A | 257 | 25.721 | 40.622 | 58.746 | 1.00 | 23.85 | AAAA |
| ATOM | 2043 | CB | THR | A | 257 | 26.460 | 41.968 | 58.549 | 1.00 | 23.99 | AAAA |
| ATOM | 2044 | CG1 | THR | A | 257 | 26.729 | 42.169 | 57.153 | 1.00 | 25.54 | AAAA |
| ATOM | 2045 | CG2 | THR | A | 257 | 27.780 | 41.985 | 59.329 | 1.00 | 24.07 | AAAA |
| ATOM | 2046 | C | THR | A | 257 | 24.438 | 40.691 | 57.948 | 1.00 | 24.97 | AAAA |

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Figure 19-32

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2047 | O | THR | A | 257 | 23.692 | 41.672 | 58.048 | 1.00 | 25.84 | AAAA |
| ATOM | 2048 | N | ASP | A | 258 | 24.152 | 39.665 | 57.154 | 1.00 | 25.18 | AAAA |
| ATOM | 2049 | CA | ASP | A | 258 | 22.935 | 39.753 | 56.379 | 1.00 | 26.18 | AAAA |
| ATOM | 2050 | CB | ASP | A | 258 | 22.950 | 38.830 | 55.149 | 1.00 | 25.52 | AAAA |
| ATOM | 2051 | CG | ASP | A | 258 | 23.211 | 37.392 | 55.494 | 1.00 | 26.33 | AAAA |
| ATOM | 2052 | C | ASP | A | 258 | 21.649 | 39.574 | 57.178 | 1.00 | 26.74 | AAAA |
| ATOM | 2053 | O | ASP | A | 258 | 20.571 | 39.823 | 56.643 | 1.00 | 26.57 | AAAA |
| ATOM | 2054 | OD1 | ASP | A | 258 | 23.014 | 37.029 | 56.675 | 1.00 | 26.85 | AAAA |
| ATOM | 2055 | OD2 | ASP | A | 258 | 23.585 | 36.623 | 54.572 | 1.00 | 24.06 | AAAA |
| ATOM | 2056 | N | PRO | A | 259 | 21.727 | 39.114 | 58.449 | 1.00 | 26.95 | AAAA |
| ATOM | 2057 | CD | PRO | A | 259 | 22.834 | 38.589 | 59.271 | 1.00 | 27.34 | AAAA |
| ATOM | 2058 | CA | PRO | A | 259 | 20.467 | 38.976 | 59.190 | 1.00 | 27.05 | AAAA |
| ATOM | 2059 | CB | PRO | A | 259 | 20.886 | 38.186 | 60.425 | 1.00 | 26.38 | AAAA |
| ATOM | 2060 | CG | PRO | A | 259 | 22.247 | 38.718 | 60.669 | 1.00 | 27.84 | AAAA |
| ATOM | 2061 | C | PRO | A | 259 | 19.914 | 40.365 | 59.543 | 1.00 | 27.32 | AAAA |
| ATOM | 2062 | O | PRO | A | 259 | 18.739 | 40.510 | 59.871 | 1.00 | 27.29 | AAAA |
| ATOM | 2063 | N | LEU | A | 260 | 20.771 | 41.383 | 59.452 | 1.00 | 26.97 | AAAA |
| ATOM | 2064 | CA | LEU | A | 260 | 20.389 | 42.763 | 59.752 | 1.00 | 26.74 | AAAA |
| ATOM | 2065 | CB | LEU | A | 260 | 21.621 | 43.680 | 59.680 | 1.00 | 27.21 | AAAA |
| ATOM | 2066 | CG | LEU | A | 260 | 22.732 | 43.465 | 60.709 | 1.00 | 27.01 | AAAA |
| ATOM | 2067 | CD1 | LEU | A | 260 | 23.889 | 44.380 | 60.408 | 1.00 | 25.51 | AAAA |
| ATOM | 2068 | CD2 | LEU | A | 260 | 22.189 | 43.718 | 62.112 | 1.00 | 27.39 | AAAA |
| ATOM | 2069 | C | LEU | A | 260 | 19.295 | 43.351 | 58.865 | 1.00 | 26.47 | AAAA |
| ATOM | 2070 | O | LEU | A | 260 | 19.278 | 43.137 | 57.649 | 1.00 | 26.72 | AAAA |
| ATOM | 2071 | N | LEU | A | 261 | 18.413 | 44.126 | 59.494 | 1.00 | 26.32 | AAAA |
| ATOM | 2072 | CA | LEU | A | 261 | 17.283 | 44.808 | 58.846 | 1.00 | 27.20 | AAAA |
| ATOM | 2073 | CB | LEU | A | 261 | 16.732 | 45.885 | 59.780 | 1.00 | 28.71 | AAAA |
| ATOM | 2074 | CG | LEU | A | 261 | 15.644 | 46.789 | 59.190 | 1.00 | 29.24 | AAAA |
| ATOM | 2075 | CD1 | LEU | A | 261 | 14.433 | 45.954 | 58.883 | 1.00 | 29.44 | AAAA |
| ATOM | 2076 | CD2 | LEU | A | 261 | 15.284 | 47.906 | 60.162 | 1.00 | 29.72 | AAAA |
| ATOM | 2077 | C | LEU | A | 261 | 17.506 | 45.454 | 57.473 | 1.00 | 27.90 | AAAA |
| ATOM | 2078 | O | LEU | A | 261 | 16.675 | 45.294 | 56.577 | 1.00 | 28.21 | AAAA |
| ATOM | 2079 | N | GLU | A | 262 | 18.597 | 46.202 | 57.310 | 1.00 | 27.61 | AAAA |
| ATOM | 2080 | CA | GLU | A | 262 | 18.887 | 46.877 | 56.043 | 1.00 | 26.92 | AAAA |
| ATOM | 2081 | CB | GLU | A | 262 | 19.949 | 47.955 | 56.241 | 1.00 | 25.85 | AAAA |
| ATOM | 2082 | CG | GLU | A | 262 | 19.549 | 49.119 | 57.117 | 1.00 | 25.36 | AAAA |
| ATOM | 2083 | CD | GLU | A | 262 | 19.552 | 48.787 | 58.580 | 1.00 | 25.78 | AAAA |
| ATOM | 2084 | OE1 | GLU | A | 262 | 19.859 | 47.631 | 58.938 | 1.00 | 24.64 | AAAA |
| ATOM | 2085 | OE2 | GLU | A | 262 | 19.255 | 49.694 | 59.381 | 1.00 | 25.82 | AAAA |
| ATOM | 2086 | C | GLU | A | 262 | 19.346 | 45.995 | 54.882 | 1.00 | 28.79 | AAAA |
| ATOM | 2087 | O | GLU | A | 262 | 19.354 | 46.439 | 53.724 | 1.00 | 28.70 | AAAA |
| ATOM | 2088 | N | ASP | A | 263 | 19.743 | 44.758 | 55.179 | 1.00 | 29.57 | AAAA |
| ATOM | 2089 | CA | ASP | A | 263 | 20.230 | 43.853 | 54.145 | 1.00 | 28.99 | AAAA |
| ATOM | 2090 | CB | ASP | A | 263 | 21.160 | 42.802 | 54.760 | 1.00 | 27.89 | AAAA |
| ATOM | 2091 | CG | ASP | A | 263 | 21.986 | 42.062 | 53.714 | 1.00 | 29.02 | AAAA |
| ATOM | 2092 | OD1 | ASP | A | 263 | 23.194 | 41.863 | 53.957 | 1.00 | 28.06 | AAAA |
| ATOM | 2093 | OD2 | ASP | A | 263 | 21.438 | 41.663 | 52.660 | 1.00 | 28.80 | AAAA |
| ATOM | 2094 | C | ASP | A | 263 | 19.066 | 43.197 | 53.431 | 1.00 | 29.73 | AAAA |
| ATOM | 2095 | O | ASP | A | 263 | 18.258 | 42.510 | 54.043 | 1.00 | 29.15 | AAAA |
| ATOM | 2096 | N | TYR | A | 264 | 19.002 | 43.416 | 52.122 | 1.00 | 31.25 | AAAA |
| ATOM | 2097 | CA | TYR | A | 264 | 17.925 | 42.888 | 51.306 | 1.00 | 32.43 | AAAA |
| ATOM | 2098 | CB | TYR | A | 264 | 17.913 | 43.558 | 49.938 | 1.00 | 34.53 | AAAA |
| ATOM | 2099 | CG | TYR | A | 264 | 17.627 | 45.038 | 49.997 | 1.00 | 38.21 | AAAA |
| ATOM | 2100 | CD1 | TYR | A | 264 | 18.664 | 45.968 | 49.983 | 1.00 | 39.87 | AAAA |
| ATOM | 2101 | CE1 | TYR | A | 264 | 18.409 | 47.335 | 50.068 | 1.00 | 41.74 | AAAA |
| ATOM | 2102 | CD2 | TYR | A | 264 | 16.316 | 45.511 | 50.103 | 1.00 | 40.10 | AAAA |
| ATOM | 2103 | CE2 | TYR | A | 264 | 16.044 | 46.877 | 50.191 | 1.00 | 41.50 | AAAA |
| ATOM | 2104 | CZ | TYR | A | 264 | 17.095 | 47.786 | 50.170 | 1.00 | 42.75 | AAAA |
| ATOM | 2105 | OH | TYR | A | 264 | 16.838 | 49.147 | 50.231 | 1.00 | 44.65 | AAAA |
| ATOM | 2106 | C | TYR | A | 264 | 17.897 | 41.385 | 51.135 | 1.00 | 32.50 | AAAA |
| ATOM | 2107 | O | TYR | A | 264 | 16.819 | 40.816 | 50.968 | 1.00 | 32.49 | AAAA |
| ATOM | 2108 | N | LEU | A | 265 | 19.064 | 40.740 | 51.171 | 1.00 | 32.64 | AAAA |
| ATOM | 2109 | CA | LEU | A | 265 | 19.122 | 39.281 | 51.036 | 1.00 | 31.92 | AAAA |
| ATOM | 2110 | CB | LEU | A | 265 | 20.525 | 38.823 | 50.617 | 1.00 | 32.75 | AAAA |
| ATOM | 2111 | CG | LEU | A | 265 | 20.808 | 39.010 | 49.127 | 1.00 | 32.95 | AAAA |
| ATOM | 2112 | CD1 | LEU | A | 265 | 22.213 | 38.588 | 48.771 | 1.00 | 31.59 | AAAA |

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Figure 19-33

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2113 | CD2 | LEU | A | 265 | 19.803 | 38.166 | 48.361 | 1.00 | 34.62 | AAAA |
| ATOM | 2114 | C | LEU | A | 265 | 18.693 | 38.540 | 52.296 | 1.00 | 30.33 | AAAA |
| ATOM | 2115 | O | LEU | A | 265 | 19.024 | 37.375 | 52.484 | 1.00 | 30.30 | AAAA |
| ATOM | 2116 | N | SER | A | 266 | 17.945 | 39.230 | 53.147 | 1.00 | 29.23 | AAAA |
| ATOM | 2117 | CA | SER | A | 266 | 17.434 | 38.649 | 54.371 | 1.00 | 29.72 | AAAA |
| ATOM | 2118 | CB | SER | A | 266 | 18.398 | 38.894 | 55.519 | 1.00 | 32.09 | AAAA |
| ATOM | 2119 | OG | SER | A | 266 | 17.728 | 38.810 | 56.771 | 1.00 | 33.43 | AAAA |
| ATOM | 2120 | C | SER | A | 266 | 16.115 | 39.290 | 54.698 | 1.00 | 28.71 | AAAA |
| ATOM | 2121 | O | SER | A | 266 | 15.924 | 40.473 | 54.444 | 1.00 | 29.67 | AAAA |
| ATOM | 2122 | N | LYS | A | 267 | 15.209 | 38.517 | 55.276 | 1.00 | 27.82 | AAAA |
| ATOM | 2123 | CA | LYS | A | 267 | 13.908 | 39.045 | 55.654 | 1.00 | 27.56 | AAAA |
| ATOM | 2124 | CB | LYS | A | 267 | 12.821 | 38.076 | 55.222 | 1.00 | 28.75 | AAAA |
| ATOM | 2125 | CG | LYS | A | 267 | 12.733 | 37.922 | 53.718 | 1.00 | 29.67 | AAAA |
| ATOM | 2126 | CD | LYS | A | 267 | 12.343 | 39.223 | 53.053 | 1.00 | 30.13 | AAAA |
| ATOM | 2127 | CE | LYS | A | 267 | 12.303 | 39.036 | 51.546 | 1.00 | 31.86 | AAAA |
| ATOM | 2128 | NZ | LYS | A | 267 | 11.796 | 40.252 | 50.843 | 1.00 | 33.92 | AAAA |
| ATOM | 2129 | C | LYS | A | 267 | 13.800 | 39.327 | 57.152 | 1.00 | 27.18 | AAAA |
| ATOM | 2130 | O | LYS | A | 267 | 12.707 | 39.591 | 57.665 | 1.00 | 27.18 | AAAA |
| ATOM | 2131 | N | PHE | A | 268 | 14.944 | 39.267 | 57.836 | 1.00 | 26.12 | AAAA |
| ATOM | 2132 | CA | PHE | A | 268 | 15.048 | 39.532 | 59.271 | 1.00 | 25.72 | AAAA |
| ATOM | 2133 | CB | PHE | A | 268 | 16.272 | 38.830 | 59.856 | 1.00 | 24.94 | AAAA |
| ATOM | 2134 | CG | PHE | A | 268 | 16.167 | 37.334 | 59.896 | 1.00 | 25.07 | AAAA |
| ATOM | 2135 | CD1 | PHE | A | 268 | 17.271 | 36.565 | 60.267 | 1.00 | 24.56 | AAAA |
| ATOM | 2136 | CD2 | PHE | A | 268 | 14.955 | 36.687 | 59.629 | 1.00 | 23.76 | AAAA |
| ATOM | 2137 | CE1 | PHE | A | 268 | 17.174 | 35.169 | 60.384 | 1.00 | 23.71 | AAAA |
| ATOM | 2138 | CE2 | PHE | A | 268 | 14.850 | 35.303 | 59.739 | 1.00 | 23.86 | AAAA |
| ATOM | 2139 | CZ | PHE | A | 268 | 15.966 | 34.542 | 60.121 | 1.00 | 23.68 | AAAA |
| ATOM | 2140 | C | PHE | A | 268 | 15.190 | 41.030 | 59.513 | 1.00 | 25.77 | AAAA |
| ATOM | 2141 | O | PHE | A | 268 | 15.811 | 41.734 | 58.726 | 1.00 | 25.81 | AAAA |
| ATOM | 2142 | N | ASN | A | 269 | 14.606 | 41.524 | 60.595 | 1.00 | 26.02 | AAAA |
| ATOM | 2143 | CA | ASN | A | 269 | 14.718 | 42.943 | 60.890 | 1.00 | 26.58 | AAAA |
| ATOM | 2144 | CB | ASN | A | 269 | 13.330 | 43.584 | 61.058 | 1.00 | 25.47 | AAAA |
| ATOM | 2145 | CG | ASN | A | 269 | 12.379 | 43.252 | 59.906 | 1.00 | 25.37 | AAAA |
| ATOM | 2146 | OD1 | ASN | A | 269 | 12.761 | 43.260 | 58.734 | 1.00 | 23.82 | AAAA |
| ATOM | 2147 | ND2 | ASN | A | 269 | 11.123 | 42.985 | 60.245 | 1.00 | 24.03 | AAAA |
| ATOM | 2148 | C | ASN | A | 269 | 15.540 | 43.112 | 62.169 | 1.00 | 26.82 | AAAA |
| ATOM | 2149 | O | ASN | A | 269 | 15.089 | 43.715 | 63.150 | 1.00 | 27.98 | AAAA |
| ATOM | 2150 | N | LEU | A | 270 | 16.744 | 42.559 | 62.149 | 1.00 | 26.07 | AAAA |
| ATOM | 2151 | CA | LEU | A | 270 | 17.639 | 42.642 | 63.289 | 1.00 | 25.97 | AAAA |
| ATOM | 2152 | CB | LEU | A | 270 | 18.634 | 41.479 | 63.265 | 1.00 | 23.76 | AAAA |
| ATOM | 2153 | CG | LEU | A | 270 | 18.048 | 40.070 | 63.225 | 1.00 | 23.36 | AAAA |
| ATOM | 2154 | CD1 | LEU | A | 270 | 19.115 | 39.090 | 63.710 | 1.00 | 21.90 | AAAA |
| ATOM | 2155 | CD2 | LEU | A | 270 | 16.824 | 39.971 | 64.122 | 1.00 | 22.05 | AAAA |
| ATOM | 2156 | C | LEU | A | 270 | 18.420 | 43.961 | 63.360 | 1.00 | 27.13 | AAAA |
| ATOM | 2157 | O | LEU | A | 270 | 18.475 | 44.750 | 62.399 | 1.00 | 25.99 | AAAA |
| ATOM | 2158 | N | SER | A | 271 | 19.038 | 44.176 | 64.517 | 1.00 | 27.97 | AAAA |
| ATOM | 2159 | CA | SER | A | 271 | 19.832 | 45.370 | 64.767 | 1.00 | 27.95 | AAAA |
| ATOM | 2160 | CB | SER | A | 271 | 19.235 | 46.137 | 65.943 | 1.00 | 27.32 | AAAA |
| ATOM | 2161 | OG | SER | A | 271 | 19.184 | 45.297 | 67.089 | 1.00 | 27.90 | AAAA |
| ATOM | 2162 | C | SER | A | 271 | 21.276 | 44.987 | 65.084 | 1.00 | 28.15 | AAAA |
| ATOM | 2163 | O | SER | A | 271 | 21.574 | 43.832 | 65.401 | 1.00 | 26.99 | AAAA |
| ATOM | 2164 | N | ASN | A | 272 | 22.156 | 45.980 | 64.979 | 1.00 | 28.96 | AAAA |
| ATOM | 2165 | CA | ASN | A | 272 | 23.590 | 45.861 | 65.266 | 1.00 | 29.54 | AAAA |
| ATOM | 2166 | CB | ASN | A | 272 | 24.247 | 47.243 | 65.223 | 1.00 | 30.96 | AAAA |
| ATOM | 2167 | CG | ASN | A | 272 | 24.647 | 47.640 | 63.850 | 1.00 | 31.20 | AAAA |
| ATOM | 2168 | OD1 | ASN | A | 272 | 24.960 | 48.794 | 63.594 | 1.00 | 31.73 | AAAA |
| ATOM | 2169 | ND2 | ASN | A | 272 | 24.670 | 46.674 | 62.948 | 1.00 | 31.93 | AAAA |
| ATOM | 2170 | C | ASN | A | 272 | 23.821 | 45.309 | 66.645 | 1.00 | 29.63 | AAAA |
| ATOM | 2171 | O | ASN | A | 272 | 24.574 | 44.361 | 66.843 | 1.00 | 29.85 | AAAA |
| ATOM | 2172 | N | VAL | A | 273 | 23.180 | 45.959 | 67.600 | 1.00 | 29.77 | AAAA |
| ATOM | 2173 | CA | VAL | A | 273 | 23.290 | 45.602 | 68.994 | 1.00 | 30.89 | AAAA |
| ATOM | 2174 | CB | VAL | A | 273 | 22.436 | 46.576 | 69.816 | 1.00 | 31.61 | AAAA |
| ATOM | 2175 | CG1 | VAL | A | 273 | 22.716 | 46.403 | 71.293 | 1.00 | 33.17 | AAAA |
| ATOM | 2176 | CG2 | VAL | A | 273 | 22.740 | 47.998 | 69.372 | 1.00 | 31.82 | AAAA |
| ATOM | 2177 | C | VAL | A | 273 | 22.883 | 44.144 | 69.266 | 1.00 | 30.74 | AAAA |
| ATOM | 2178 | O | VAL | A | 273 | 23.550 | 43.431 | 70.022 | 1.00 | 31.23 | AAAA |

SUBSTITUTE SHEET (RULE 26)

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Figure 19-34

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2179 | N | ALA | A | 274 | 21.785 | 43.706 | 68.659 | 1.00 | 30.25 | AAAA |
| ATOM | 2180 | CA | ALA | A | 274 | 21.327 | 42.333 | 68.840 | 1.00 | 29.87 | AAAA |
| ATOM | 2181 | CB | ALA | A | 274 | 20.005 | 42.119 | 68.112 | 1.00 | 29.64 | AAAA |
| ATOM | 2182 | C | ALA | A | 274 | 22.395 | 41.438 | 68.247 | 1.00 | 29.35 | AAAA |
| ATOM | 2183 | O | ALA | A | 274 | 22.707 | 40.373 | 68.778 | 1.00 | 29.18 | AAAA |
| ATOM | 2184 | N | PHE | A | 275 | 22.946 | 41.893 | 67.127 | 1.00 | 29.30 | AAAA |
| ATOM | 2185 | CA | PHE | A | 275 | 23.991 | 41.170 | 66.428 | 1.00 | 28.91 | AAAA |
| ATOM | 2186 | CB | PHE | A | 275 | 24.375 | 41.909 | 65.150 | 1.00 | 28.77 | AAAA |
| ATOM | 2187 | CG | PHE | A | 275 | 25.354 | 41.170 | 64.308 | 1.00 | 28.08 | AAAA |
| ATOM | 2188 | CD1 | PHE | A | 275 | 25.015 | 39.954 | 63.740 | 1.00 | 28.92 | AAAA |
| ATOM | 2189 | CD2 | PHE | A | 275 | 26.621 | 41.684 | 64.077 | 1.00 | 29.48 | AAAA |
| ATOM | 2190 | CE1 | PHE | A | 275 | 25.928 | 39.259 | 62.945 | 1.00 | 29.20 | AAAA |
| ATOM | 2191 | CE2 | PHE | A | 275 | 27.546 | 40.988 | 63.279 | 1.00 | 29.24 | AAAA |
| ATOM | 2192 | CZ | PHE | A | 275 | 27.193 | 39.779 | 62.716 | 1.00 | 28.30 | AAAA |
| ATOM | 2193 | C | PHE | A | 275 | 25.196 | 41.058 | 67.351 | 1.00 | 27.64 | AAAA |
| ATOM | 2194 | O | PHE | A | 275 | 25.728 | 39.975 | 67.558 | 1.00 | 28.65 | AAAA |
| ATOM | 2195 | N | LEU | A | 276 | 25.606 | 42.189 | 67.902 | 1.00 | 26.81 | AAAA |
| ATOM | 2196 | CA | LEU | A | 276 | 26.732 | 42.260 | 68.831 | 1.00 | 27.38 | AAAA |
| ATOM | 2197 | CB | LEU | A | 276 | 26.878 | 43.700 | 69.353 | 1.00 | 27.53 | AAAA |
| ATOM | 2198 | CG | LEU | A | 276 | 28.202 | 44.213 | 69.928 | 1.00 | 26.37 | AAAA |
| ATOM | 2199 | CD1 | LEU | A | 276 | 27.923 | 45.488 | 70.721 | 1.00 | 25.71 | AAAA |
| ATOM | 2200 | CD2 | LEU | A | 276 | 28.842 | 43.189 | 70.827 | 1.00 | 27.06 | AAAA |
| ATOM | 2201 | C | LEU | A | 276 | 26.486 | 41.317 | 70.021 | 1.00 | 26.49 | AAAA |
| ATOM | 2202 | O | LEU | A | 276 | 27.387 | 40.603 | 70.471 | 1.00 | 25.26 | AAAA |
| ATOM | 2203 | N | LYS | A | 277 | 25.257 | 41.322 | 70.524 | 1.00 | 27.46 | AAAA |
| ATOM | 2204 | CA | LYS | A | 277 | 24.894 | 40.468 | 71.642 | 1.00 | 28.63 | AAAA |
| ATOM | 2205 | CB | LYS | A | 277 | 23.542 | 40.862 | 72.223 | 1.00 | 30.63 | AAAA |
| ATOM | 2206 | CG | LYS | A | 277 | 23.590 | 42.029 | 73.153 | 1.00 | 33.14 | AAAA |
| ATOM | 2207 | CD | LYS | A | 277 | 22.599 | 41.791 | 74.268 | 1.00 | 34.94 | AAAA |
| ATOM | 2208 | CE | LYS | A | 277 | 22.964 | 40.519 | 75.029 | 1.00 | 36.17 | AAAA |
| ATOM | 2209 | NZ | LYS | A | 277 | 21.979 | 40.194 | 76.104 | 1.00 | 38.64 | AAAA |
| ATOM | 2210 | C | LYS | A | 277 | 24.846 | 38.997 | 71.297 | 1.00 | 28.53 | AAAA |
| ATOM | 2211 | O | LYS | A | 277 | 25.118 | 38.152 | 72.146 | 1.00 | 28.45 | AAAA |
| ATOM | 2212 | N | ALA | A | 278 | 24.466 | 38.681 | 70.064 | 1.00 | 28.47 | AAAA |
| ATOM | 2213 | CA | ALA | A | 278 | 24.404 | 37.280 | 69.656 | 1.00 | 27.66 | AAAA |
| ATOM | 2214 | CB | ALA | A | 278 | 23.941 | 37.181 | 68.201 | 1.00 | 26.40 | AAAA |
| ATOM | 2215 | C | ALA | A | 278 | 25.833 | 36.754 | 69.820 | 1.00 | 26.63 | AAAA |
| ATOM | 2216 | O | ALA | A | 278 | 26.081 | 35.644 | 70.317 | 1.00 | 25.19 | AAAA |
| ATOM | 2217 | N | PHE | A | 279 | 26.764 | 37.616 | 69.427 | 1.00 | 26.50 | AAAA |
| ATOM | 2218 | CA | PHE | A | 279 | 28.181 | 37.345 | 69.481 | 1.00 | 25.83 | AAAA |
| ATOM | 2219 | CB | PHE | A | 279 | 28.934 | 38.521 | 68.869 | 1.00 | 26.35 | AAAA |
| ATOM | 2220 | CG | PHE | A | 279 | 30.413 | 38.319 | 68.796 | 1.00 | 27.92 | AAAA |
| ATOM | 2221 | CD1 | PHE | A | 279 | 30.949 | 37.256 | 68.072 | 1.00 | 28.58 | AAAA |
| ATOM | 2222 | CD2 | PHE | A | 279 | 31.280 | 39.201 | 69.434 | 1.00 | 28.33 | AAAA |
| ATOM | 2223 | CE1 | PHE | A | 279 | 32.330 | 37.078 | 67.983 | 1.00 | 28.22 | AAAA |
| ATOM | 2224 | CE2 | PHE | A | 279 | 32.666 | 39.030 | 69.349 | 1.00 | 28.11 | AAAA |
| ATOM | 2225 | CZ | PHE | A | 279 | 33.185 | 37.968 | 68.622 | 1.00 | 28.21 | AAAA |
| ATOM | 2226 | C | PHE | A | 279 | 28.665 | 37.118 | 70.901 | 1.00 | 25.47 | AAAA |
| ATOM | 2227 | O | PHE | A | 279 | 29.284 | 36.091 | 71.202 | 1.00 | 24.32 | AAAA |
| ATOM | 2228 | N | ASN | A | 280 | 28.382 | 38.075 | 71.778 | 1.00 | 25.12 | AAAA |
| ATOM | 2229 | CA | ASN | A | 280 | 28.841 | 37.944 | 73.147 | 1.00 | 25.05 | AAAA |
| ATOM | 2230 | CB | ASN | A | 280 | 28.708 | 39.269 | 73.887 | 1.00 | 24.42 | AAAA |
| ATOM | 2231 | CG | ASN | A | 280 | 29.683 | 40.300 | 73.364 | 1.00 | 24.56 | AAAA |
| ATOM | 2232 | OD1 | ASN | A | 280 | 30.841 | 39.980 | 73.080 | 1.00 | 23.24 | AAAA |
| ATOM | 2233 | ND2 | ASN | A | 280 | 29.233 | 41.543 | 73.249 | 1.00 | 24.59 | AAAA |
| ATOM | 2234 | C | ASN | A | 280 | 28.213 | 36.814 | 73.925 | 1.00 | 24.79 | AAAA |
| ATOM | 2235 | O | ASN | A | 280 | 28.828 | 36.272 | 74.825 | 1.00 | 24.96 | AAAA |
| ATOM | 2236 | N | ILE | A | 281 | 26.998 | 36.444 | 73.565 | 1.00 | 24.87 | AAAA |
| ATOM | 2237 | CA | ILE | A | 281 | 26.332 | 35.337 | 74.220 | 1.00 | 24.80 | AAAA |
| ATOM | 2238 | CB | ILE | A | 281 | 24.866 | 35.252 | 73.780 | 1.00 | 24.40 | AAAA |
| ATOM | 2239 | CG2 | ILE | A | 281 | 24.297 | 33.907 | 74.124 | 1.00 | 25.03 | AAAA |
| ATOM | 2240 | CG1 | ILE | A | 281 | 24.076 | 36.386 | 74.424 | 1.00 | 24.70 | AAAA |
| ATOM | 2241 | CD1 | ILE | A | 281 | 22.613 | 36.379 | 74.069 | 1.00 | 26.49 | AAAA |
| ATOM | 2242 | C | ILE | A | 281 | 27.044 | 34.027 | 73.884 | 1.00 | 25.21 | AAAA |
| ATOM | 2243 | O | ILE | A | 281 | 27.220 | 33.170 | 74.750 | 1.00 | 24.97 | AAAA |
| ATCM | 2244 | N | VAL | A | 282 | 27.440 | 33.866 | 72.620 | 1.00 | 25.98 | AAAA |

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Figure 19-35

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2245 | CA | VAL | A | 282 | 28.150 | 32.656 | 72.193 | 1.00 | 25.15 | AAAA |
| ATOM | 2246 | CB | VAL | A | 282 | 28.451 | 32.666 | 70.677 | 1.00 | 23.83 | AAAA |
| ATOM | 2247 | CG1 | VAL | A | 282 | 29.315 | 31.470 | 70.311 | 1.00 | 23.58 | AAAA |
| ATOM | 2248 | CG2 | VAL | A | 282 | 27.173 | 32.633 | 69.899 | 1.00 | 22.73 | AAAA |
| ATOM | 2249 | C | VAL | A | 282 | 29.478 | 32.553 | 72.936 | 1.00 | 25.73 | AAAA |
| ATOM | 2250 | O | VAL | A | 282 | 29.928 | 31.457 | 73.275 | 1.00 | 25.31 | AAAA |
| ATOM | 2251 | N | ARG | A | 283 | 30.100 | 33.702 | 73.176 | 1.00 | 26.90 | AAAA |
| ATOM | 2252 | CA | ARG | A | 283 | 31.372 | 33.760 | 73.885 | 1.00 | 28.87 | AAAA |
| ATOM | 2253 | CB | ARG | A | 283 | 32.027 | 35.131 | 73.684 | 1.00 | 28.16 | AAAA |
| ATOM | 2254 | CG | ARG | A | 283 | 32.364 | 35.440 | 72.240 | 1.00 | 27.22 | AAAA |
| ATOM | 2255 | CD | ARG | A | 283 | 32.821 | 36.862 | 72.098 | 1.00 | 27.08 | AAAA |
| ATOM | 2256 | NE | ARG | A | 283 | 34.035 | 37.116 | 72.854 | 1.00 | 26.73 | AAAA |
| ATOM | 2257 | CZ | ARG | A | 283 | 34.514 | 38.327 | 73.091 | 1.00 | 26.82 | AAAA |
| ATOM | 2258 | NH1 | ARG | A | 283 | 33.873 | 39.384 | 72.626 | 1.00 | 27.36 | AAAA |
| ATOM | 2259 | NH2 | ARG | A | 283 | 35.622 | 38.484 | 73.798 | 1.00 | 26.95 | AAAA |
| ATOM | 2260 | C | ARG | A | 283 | 31.183 | 33.494 | 75.376 | 1.00 | 30.71 | AAAA |
| ATOM | 2261 | O | ARG | A | 283 | 32.086 | 32.981 | 76.027 | 1.00 | 30.68 | AAAA |
| ATOM | 2262 | N | GLU | A | 284 | 30.014 | 33.842 | 75.911 | 1.00 | 32.71 | AAAA |
| ATOM | 2263 | CA | GLU | A | 284 | 29.735 | 33.623 | 77.323 | 1.00 | 35.53 | AAAA |
| ATOM | 2264 | CB | GLU | A | 284 | 28.482 | 34.391 | 77.751 | 1.00 | 37.39 | AAAA |
| ATOM | 2265 | CG | GLU | A | 284 | 28.538 | 35.854 | 77.392 | 1.00 | 41.73 | AAAA |
| ATOM | 2266 | CD | GLU | A | 284 | 27.272 | 36.631 | 77.754 | 1.00 | 45.27 | AAAA |
| ATOM | 2267 | OE1 | GLU | A | 284 | 26.151 | 36.078 | 77.610 | 1.00 | 46.66 | AAAA |
| ATOM | 2268 | OE2 | GLU | A | 284 | 27.405 | 37.817 | 78.148 | 1.00 | 46.94 | AAAA |
| ATOM | 2269 | C | GLU | A | 284 | 29.524 | 32.133 | 77.564 | 1.00 | 36.25 | AAAA |
| ATOM | 2270 | O | GLU | A | 284 | 29.920 | 31.593 | 78.601 | 1.00 | 37.85 | AAAA |
| ATOM | 2271 | N | VAL | A | 285 | 28.916 | 31.464 | 76.591 | 1.00 | 35.24 | AAAA |
| ATOM | 2272 | CA | VAL | A | 285 | 28.637 | 30.041 | 76.708 | 1.00 | 33.88 | AAAA |
| ATOM | 2273 | CB | VAL | A | 285 | 27.505 | 29.619 | 75.737 | 1.00 | 33.71 | AAAA |
| ATOM | 2274 | CG1 | VAL | A | 285 | 27.201 | 28.137 | 75.888 | 1.00 | 32.59 | AAAA |
| ATOM | 2275 | CG2 | VAL | A | 285 | 26.254 | 30.457 | 76.001 | 1.00 | 32.77 | AAAA |
| ATOM | 2276 | C | VAL | A | 285 | 29.847 | 29.149 | 76.456 | 1.00 | 33.47 | AAAA |
| ATOM | 2277 | O | VAL | A | 285 | 30.140 | 28.262 | 77.257 | 1.00 | 34.23 | AAAA |
| ATOM | 2278 | N | PHE | A | 286 | 30.568 | 29.389 | 75.364 | 1.00 | 32.34 | AAAA |
| ATOM | 2279 | CA | PHE | A | 286 | 31.706 | 28.535 | 75.036 | 1.00 | 29.92 | AAAA |
| ATOM | 2280 | CB | PHE | A | 286 | 31.533 | 27.960 | 73.635 | 1.00 | 29.77 | AAAA |
| ATOM | 2281 | CG | PHE | A | 286 | 30.267 | 27.179 | 73.444 | 1.00 | 28.64 | AAAA |
| ATOM | 2282 | CD1 | PHE | A | 286 | 29.152 | 27.772 | 72.863 | 1.00 | 28.75 | AAAA |
| ATOM | 2283 | CD2 | PHE | A | 286 | 30.197 | 25.837 | 73.827 | 1.00 | 28.55 | AAAA |
| ATOM | 2284 | CE1 | PHE | A | 286 | 27.983 | 27.039 | 72.660 | 1.00 | 29.04 | AAAA |
| ATOM | 2285 | CE2 | PHE | A | 286 | 29.037 | 25.095 | 73.629 | 1.00 | 28.19 | AAAA |
| ATOM | 2286 | CZ | PHE | A | 286 | 27.929 | 25.694 | 73.045 | 1.00 | 28.73 | AAAA |
| ATOM | 2287 | C | PHE | A | 286 | 33.106 | 29.113 | 75.132 | 1.00 | 29.13 | AAAA |
| ATOM | 2288 | O | PHE | A | 286 | 34.073 | 28.436 | 74.760 | 1.00 | 28.54 | AAAA |
| ATOM | 2289 | N | GLY | A | 287 | 33.224 | 30.341 | 75.637 | 1.00 | 28.42 | AAAA |
| ATOM | 2290 | CA | GLY | A | 287 | 34.525 | 30.987 | 75.744 | 1.00 | 27.07 | AAAA |
| ATOM | 2291 | C | GLY | A | 287 | 34.932 | 31.611 | 74.419 | 1.00 | 26.64 | AAAA |
| ATOM | 2292 | O | GLY | A | 287 | 34.088 | 32.042 | 73.649 | 1.00 | 27.13 | AAAA |
| ATOM | 2293 | N | GLU | A | 288 | 36.227 | 31.665 | 74.146 | 1.00 | 27.20 | AAAA |
| ATOM | 2294 | CA | GLU | A | 288 | 36.719 | 32.238 | 72.900 | 1.00 | 27.52 | AAAA |
| ATOM | 2295 | CB | GLU | A | 288 | 38.073 | 32.923 | 73.108 | 1.00 | 28.18 | AAAA |
| ATOM | 2296 | CG | GLU | A | 288 | 38.036 | 34.177 | 73.959 | 1.00 | 28.88 | AAAA |
| ATOM | 2297 | CD | GLU | A | 288 | 37.329 | 35.330 | 73.279 | 1.00 | 29.58 | AAAA |
| ATOM | 2298 | OE1 | GLU | A | 288 | 37.807 | 35.813 | 72.243 | 1.00 | 29.94 | AAAA |
| ATOM | 2299 | OE2 | GLU | A | 288 | 36.281 | 35.761 | 73.782 | 1.00 | 31.89 | AAAA |
| ATOM | 2300 | C | GLU | A | 288 | 36.877 | 31.158 | 71.843 | 1.00 | 27.44 | AAAA |
| ATOM | 2301 | O | GLU | A | 288 | 37.169 | 30.007 | 72.162 | 1.00 | 27.87 | AAAA |
| ATOM | 2302 | N | GLY | A | 289 | 36.663 | 31.547 | 70.589 | 1.00 | 26.55 | AAAA |
| ATOM | 2303 | CA | GLY | A | 289 | 36.795 | 30.638 | 69.466 | 1.00 | 25.25 | AAAA |
| ATOM | 2304 | C | GLY | A | 289 | 37.285 | 31.414 | 68.254 | 1.00 | 24.56 | AAAA |
| ATOM | 2305 | O | GLY | A | 289 | 37.635 | 32.586 | 68.369 | 1.00 | 24.40 | AAAA |
| ATOM | 2306 | N | VAL | A | 290 | 37.320 | 30.765 | 67.095 | 1.00 | 24.04 | AAAA |
| ATOM | 2307 | CA | VAL | A | 290 | 37.756 | 31.407 | 65.863 | 1.00 | 23.76 | AAAA |
| ATOM | 2308 | CB | VAL | A | 290 | 38.288 | 30.346 | 64.867 | 1.00 | 24.94 | AAAA |
| ATOM | 2309 | CG1 | VAL | A | 290 | 38.835 | 31.012 | 63.596 | 1.00 | 22.73 | AAAA |
| ATOM | 2310 | CG2 | VAL | A | 290 | 39.375 | 29.506 | 65.555 | 1.00 | 24.74 | AAAA |

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Figure 19-36

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2311 | C | VAL | A | 290 | 36.536 | 32.122 | 65.277 | 1.00 | 23.90 | AAAA |
| ATOM | 2312 | O | VAL | A | 290 | 35.497 | 31.502 | 65.100 | 1.00 | 25.15 | AAAA |
| ATOM | 2313 | N | TYR | A | 291 | 36.662 | 33.415 | 64.976 | 1.00 | 23.09 | AAAA |
| ATOM | 2314 | CA | TYR | A | 291 | 35.544 | 34.211 | 64.446 | 1.00 | 21.41 | AAAA |
| ATOM | 2315 | CB | TYR | A | 291 | 35.472 | 35.540 | 65.193 | 1.00 | 20.57 | AAAA |
| ATOM | 2316 | CG | TYR | A | 291 | 35.511 | 35.346 | 66.677 | 1.00 | 19.87 | AAAA |
| ATOM | 2317 | CD1 | TYR | A | 291 | 36.596 | 35.782 | 67.432 | 1.00 | 20.86 | AAAA |
| ATOM | 2318 | CE1 | TYR | A | 291 | 36.677 | 35.513 | 68.793 | 1.00 | 21.47 | AAAA |
| ATOM | 2319 | CD2 | TYR | A | 291 | 34.509 | 34.647 | 67.318 | 1.00 | 20.90 | AAAA |
| ATOM | 2320 | CE2 | TYR | A | 291 | 34.579 | 34.372 | 68.675 | 1.00 | 21.90 | AAAA |
| ATOM | 2321 | CZ | TYR | A | 291 | 35.661 | 34.800 | 69.403 | 1.00 | 21.25 | AAAA |
| ATOM | 2322 | OH | TYR | A | 291 | 35.737 | 34.469 | 70.730 | 1.00 | 23.75 | AAAA |
| ATOM | 2323 | C | TYR | A | 291 | 35.607 | 34.483 | 62.946 | 1.00 | 21.25 | AAAA |
| ATOM | 2324 | O | TYR | A | 291 | 36.573 | 35.077 | 62.451 | 1.00 | 21.10 | AAAA |
| ATOM | 2325 | N | LEU | A | 292 | 34.557 | 34.084 | 62.231 | 1.00 | 20.92 | AAAA |
| ATOM | 2326 | CA | LEU | A | 292 | 34.518 | 34.260 | 60.779 | 1.00 | 20.92 | AAAA |
| ATOM | 2327 | CB | LEU | A | 292 | 34.235 | 32.916 | 60.080 | 1.00 | 19.93 | AAAA |
| ATOM | 2328 | CG | LEU | A | 292 | 35.104 | 31.688 | 60.399 | 1.00 | 17.31 | AAAA |
| ATOM | 2329 | CD1 | LEU | A | 292 | 34.685 | 30.515 | 59.528 | 1.00 | 16.05 | AAAA |
| ATOM | 2330 | CD2 | LEU | A | 292 | 36.552 | 32.000 | 60.163 | 1.00 | 18.07 | AAAA |
| ATOM | 2331 | C | LEU | A | 292 | 33.515 | 35.288 | 60.283 | 1.00 | 21.12 | AAAA |
| ATOM | 2332 | O | LEU | A | 292 | 32.652 | 35.741 | 61.020 | 1.00 | 20.70 | AAAA |
| ATOM | 2333 | N | GLY | A | 293 | 33.660 | 35.660 | 59.017 | 1.00 | 21.74 | AAAA |
| ATOM | 2334 | CA | GLY | A | 293 | 32.752 | 36.612 | 58.410 | 1.00 | 21.48 | AAAA |
| ATOM | 2335 | C | GLY | A | 293 | 31.612 | 35.856 | 57.770 | 1.00 | 21.65 | AAAA |
| ATOM | 2336 | O | GLY | A | 293 | 31.237 | 34.790 | 58.235 | 1.00 | 22.25 | AAAA |
| ATOM | 2337 | N | GLY | A | 294 | 31.060 | 36.392 | 56.691 | 1.00 | 22.66 | AAAA |
| ATOM | 2338 | CA | GLY | A | 294 | 29.957 | 35.714 | 56.034 | 1.00 | 23.61 | AAAA |
| ATOM | 2339 | C | GLY | A | 294 | 29.180 | 36.653 | 55.146 | 1.00 | 24.56 | AAAA |
| ATOM | 2340 | O | GLY | A | 294 | 29.679 | 37.727 | 54.790 | 1.00 | 25.54 | AAAA |
| ATOM | 2341 | N | GLY | A | 295 | 27.956 | 36.265 | 54.794 | 1.00 | 24.06 | AAAA |
| ATOM | 2342 | CA | GLY | A | 295 | 27.139 | 37.093 | 53.927 | 1.00 | 22.78 | AAAA |
| ATOM | 2343 | C | GLY | A | 295 | 26.902 | 38.479 | 54.483 | 1.00 | 23.11 | AAAA |
| ATOM | 2344 | O | GLY | A | 295 | 26.870 | 38.676 | 55.696 | 1.00 | 22.87 | AAAA |
| ATOM | 2345 | N | GLY | A | 296 | 26.733 | 39.442 | 53.584 | 1.00 | 22.78 | AAAA |
| ATOM | 2346 | CA | GLY | A | 296 | 26.497 | 40.813 | 53.993 | 1.00 | 23.44 | AAAA |
| ATOM | 2347 | C | GLY | A | 296 | 26.471 | 41.618 | 52.718 | 1.00 | 23.72 | AAAA |
| ATOM | 2348 | O | GLY | A | 296 | 27.474 | 41.661 | 52.004 | 1.00 | 23.73 | AAAA |
| ATOM | 2349 | N | TYR | A | 297 | 25.356 | 42.280 | 52.425 | 1.00 | 23.41 | AAAA |
| ATOM | 2350 | CA | TYR | A | 297 | 25.282 | 42.991 | 51.163 | 1.00 | 22.71 | AAAA |
| ATOM | 2351 | CB | TYR | A | 297 | 24.252 | 42.294 | 50.296 | 1.00 | 21.55 | AAAA |
| ATOM | 2352 | CG | TYR | A | 297 | 24.496 | 40.809 | 50.317 | 1.00 | 21.93 | AAAA |
| ATOM | 2353 | CD1 | TYR | A | 297 | 24.036 | 40.016 | 51.375 | 1.00 | 20.95 | AAAA |
| ATOM | 2354 | CE1 | TYR | A | 297 | 24.400 | 38.678 | 51.481 | 1.00 | 21.59 | AAAA |
| ATOM | 2355 | CD2 | TYR | A | 297 | 25.320 | 40.217 | 49.358 | 1.00 | 21.71 | AAAA |
| ATOM | 2356 | CE2 | TYR | A | 297 | 25.688 | 38.900 | 49.451 | 1.00 | 21.99 | AAAA |
| ATOM | 2357 | CZ | TYR | A | 297 | 25.242 | 38.127 | 50.511 | 1.00 | 22.18 | AAAA |
| ATOM | 2358 | OH | TYR | A | 297 | 25.721 | 36.841 | 50.615 | 1.00 | 21.35 | AAAA |
| ATOM | 2359 | C | TYR | A | 297 | 25.042 | 44.485 | 51.225 | 1.00 | 22.90 | AAAA |
| ATOM | 2360 | O | TYR | A | 297 | 25.106 | 45.172 | 50.203 | 1.00 | 23.17 | AAAA |
| ATOM | 2361 | N | HIS | A | 298 | 24.772 | 44.989 | 52.417 | 1.00 | 22.47 | AAAA |
| ATOM | 2362 | CA | HIS | A | 298 | 24.572 | 46.415 | 52.566 | 1.00 | 24.27 | AAAA |
| ATOM | 2363 | CB | HIS | A | 298 | 23.468 | 46.726 | 53.556 | 1.00 | 23.17 | AAAA |
| ATOM | 2364 | CG | HIS | A | 298 | 23.097 | 48.166 | 53.572 | 1.00 | 23.20 | AAAA |
| ATOM | 2365 | CD2 | HIS | A | 298 | 23.588 | 49.201 | 54.287 | 1.00 | 24.25 | AAAA |
| ATOM | 2366 | ND1 | HIS | A | 298 | 22.199 | 48.708 | 52.680 | 1.00 | 23.14 | AAAA |
| ATOM | 2367 | CE1 | HIS | A | 298 | 22.151 | 50.017 | 52.848 | 1.00 | 23.31 | AAAA |
| ATOM | 2368 | NE2 | HIS | A | 298 | 22.986 | 50.342 | 53.814 | 1.00 | 23.62 | AAAA |
| ATOM | 2369 | C | HIS | A | 298 | 25.886 | 46.976 | 53.106 | 1.00 | 25.17 | AAAA |
| ATOM | 2370 | O | HIS | A | 298 | 26.282 | 46.687 | 54.239 | 1.00 | 24.47 | AAAA |
| ATOM | 2371 | N | PRO | A | 299 | 26.563 | 47.818 | 52.316 | 1.00 | 26.37 | AAAA |
| ATOM | 2372 | CD | PRO | A | 299 | 26.178 | 48.372 | 51.006 | 1.00 | 27.01 | AAAA |
| ATOM | 2373 | CA | PRO | A | 299 | 27.840 | 48.394 | 52.752 | 1.00 | 27.31 | AAAA |
| ATOM | 2374 | CB | PRO | A | 299 | 28.156 | 49.383 | 51.630 | 1.00 | 27.04 | AAAA |
| ATOM | 2375 | CG | PRO | A | 299 | 26.743 | 49.764 | 51.120 | 1.00 | 27.57 | AAAA |
| ATOM | 2376 | C | PRO | A | 299 | 27.824 | 49.037 | 54.149 | 1.00 | 27.77 | AAAA |

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Figure 19-37

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2377 | O | PRO | A | 299 | 28.755 | 48.826 | 54.939 | 1.00 | 28.04 | AAAA |
| ATOM | 2378 | N | TYR | A | 300 | 26.769 | 49.794 | 54.452 | 1.00 | 27.04 | AAAA |
| ATOM | 2379 | CA | TYR | A | 300 | 26.629 | 50.477 | 55.740 | 1.00 | 27.59 | AAAA |
| ATOM | 2380 | CB | TYR | A | 300 | 25.425 | 51.437 | 55.700 | 1.00 | 30.57 | AAAA |
| ATOM | 2381 | CG | TYR | A | 300 | 25.516 | 52.599 | 54.718 | 1.00 | 32.91 | AAAA |
| ATOM | 2382 | CD1 | TYR | A | 300 | 26.181 | 52.464 | 53.491 | 1.00 | 33.45 | AAAA |
| ATOM | 2383 | CE1 | TYR | A | 300 | 26.160 | 53.487 | 52.538 | 1.00 | 33.91 | AAAA |
| ATOM | 2384 | CD2 | TYR | A | 300 | 24.837 | 53.801 | 54.969 | 1.00 | 34.19 | AAAA |
| ATOM | 2385 | CE2 | TYR | A | 300 | 24.809 | 54.830 | 54.018 | 1.00 | 34.64 | AAAA |
| ATOM | 2386 | CZ | TYR | A | 300 | 25.468 | 54.657 | 52.807 | 1.00 | 34.56 | AAAA |
| ATOM | 2387 | OH | TYR | A | 300 | 25.389 | 55.630 | 51.844 | 1.00 | 36.05 | AAAA |
| ATOM | 2388 | C | TYR | A | 300 | 26.454 | 49.538 | 56.936 | 1.00 | 26.48 | AAAA |
| ATOM | 2389 | O | TYR | A | 300 | 27.073 | 49.726 | 57.979 | 1.00 | 25.81 | AAAA |
| ATOM | 2390 | N | ALA | A | 301 | 25.581 | 48.547 | 56.791 | 1.00 | 25.41 | AAAA |
| ATOM | 2391 | CA | ALA | A | 301 | 25.328 | 47.606 | 57.865 | 1.00 | 24.64 | AAAA |
| ATOM | 2392 | CB | ALA | A | 301 | 24.164 | 46.731 | 57.511 | 1.00 | 25.32 | AAAA |
| ATOM | 2393 | C | ALA | A | 301 | 26.568 | 46.775 | 58.067 | 1.00 | 25.53 | AAAA |
| ATOM | 2394 | O | ALA | A | 301 | 27.030 | 46.567 | 59.194 | 1.00 | 26.39 | AAAA |
| ATOM | 2395 | N | LEU | A | 302 | 27.108 | 46.304 | 56.950 | 1.00 | 25.83 | AAAA |
| ATOM | 2396 | CA | LEU | A | 302 | 28.323 | 45.500 | 56.926 | 1.00 | 26.32 | AAAA |
| ATOM | 2397 | CB | LEU | A | 302 | 28.782 | 45.378 | 55.479 | 1.00 | 27.38 | AAAA |
| ATOM | 2398 | CG | LEU | A | 302 | 30.081 | 44.723 | 55.024 | 1.00 | 28.18 | AAAA |
| ATOM | 2399 | CD1 | LEU | A | 302 | 30.119 | 44.840 | 53.502 | 1.00 | 29.32 | AAAA |
| ATOM | 2400 | CD2 | LEU | A | 302 | 31.296 | 45.389 | 55.613 | 1.00 | 27.38 | AAAA |
| ATOM | 2401 | C | LEU | A | 302 | 29.398 | 46.187 | 57.764 | 1.00 | 26.41 | AAAA |
| ATOM | 2402 | O | LEU | A | 302 | 29.874 | 45.648 | 58.755 | 1.00 | 26.62 | AAAA |
| ATOM | 2403 | N | ALA | A | 303 | 29.756 | 47.397 | 57.353 | 1.00 | 26.50 | AAAA |
| ATOM | 2404 | CA | ALA | A | 303 | 30.778 | 48.176 | 58.022 | 1.00 | 25.92 | AAAA |
| ATOM | 2405 | CB | ALA | A | 303 | 31.001 | 49.475 | 57.277 | 1.00 | 25.24 | AAAA |
| ATOM | 2406 | C | ALA | A | 303 | 30.490 | 48.464 | 59.487 | 1.00 | 26.03 | AAAA |
| ATOM | 2407 | O | ALA | A | 303 | 31.325 | 48.175 | 60.340 | 1.00 | 26.95 | AAAA |
| ATOM | 2408 | N | ARG | A | 304 | 29.322 | 49.028 | 59.792 | 1.00 | 25.29 | AAAA |
| ATOM | 2409 | CA | ARG | A | 304 | 28.999 | 49.353 | 61.179 | 1.00 | 23.46 | AAAA |
| ATOM | 2410 | CB | ARG | A | 304 | 27.641 | 50.059 | 61.291 | 1.00 | 23.78 | AAAA |
| ATOM | 2411 | CG | ARG | A | 304 | 27.553 | 51.451 | 60.629 | 1.00 | 24.59 | AAAA |
| ATOM | 2412 | CD | ARG | A | 304 | 26.302 | 52.223 | 61.091 | 1.00 | 25.85 | AAAA |
| ATOM | 2413 | NE | ARG | A | 304 | 25.067 | 51.465 | 60.869 | 1.00 | 27.54 | AAAA |
| ATOM | 2414 | CZ | ARG | A | 304 | 23.978 | 51.547 | 61.637 | 1.00 | 28.36 | AAAA |
| ATOM | 2415 | NH1 | ARG | A | 304 | 23.957 | 52.362 | 62.695 | 1.00 | 26.48 | AAAA |
| ATOM | 2416 | NH2 | ARG | A | 304 | 22.910 | 50.794 | 61.358 | 1.00 | 28.45 | AAAA |
| ATOM | 2417 | C | ARG | A | 304 | 28.991 | 48.118 | 62.053 | 1.00 | 23.18 | AAAA |
| ATOM | 2418 | O | ARG | A | 304 | 29.591 | 48.099 | 63.135 | 1.00 | 22.26 | AAAA |
| ATOM | 2419 | N | ALA | A | 305 | 28.330 | 47.075 | 61.560 | 1.00 | 23.20 | AAAA |
| ATOM | 2420 | CA | ALA | A | 305 | 28.200 | 45.817 | 62.292 | 1.00 | 22.33 | AAAA |
| ATOM | 2421 | CB | ALA | A | 305 | 27.319 | 44.866 | 61.516 | 1.00 | 22.17 | AAAA |
| ATOM | 2422 | C | ALA | A | 305 | 29.516 | 45.137 | 62.621 | 1.00 | 22.27 | AAAA |
| ATOM | 2423 | O | ALA | A | 305 | 29.763 | 44.757 | 63.760 | 1.00 | 22.48 | AAAA |
| ATOM | 2424 | N | TRP | A | 306 | 30.366 | 44.969 | 61.620 | 1.00 | 22.57 | AAAA |
| ATOM | 2425 | CA | TRP | A | 306 | 31.634 | 44.307 | 61.861 | 1.00 | 21.28 | AAAA |
| ATOM | 2426 | CB | TRP | A | 306 | 32.279 | 43.885 | 60.553 | 1.00 | 21.07 | AAAA |
| ATOM | 2427 | CG | TRP | A | 306 | 31.703 | 42.618 | 60.004 | 1.00 | 20.75 | AAAA |
| ATOM | 2428 | CD2 | TRP | A | 306 | 31.886 | 42.103 | 58.683 | 1.00 | 19.54 | AAAA |
| ATOM | 2429 | CE2 | TRP | A | 306 | 31.352 | 40.795 | 58.668 | 1.00 | 19.18 | AAAA |
| ATOM | 2430 | CE3 | TRP | A | 306 | 32.456 | 42.616 | 57.510 | 1.00 | 19.59 | AAAA |
| ATOM | 2431 | CD1 | TRP | A | 306 | 31.071 | 41.632 | 60.713 | 1.00 | 20.51 | AAAA |
| ATOM | 2432 | NE1 | TRP | A | 306 | 30.864 | 40.537 | 59.922 | 1.00 | 19.74 | AAAA |
| ATOM | 2433 | CZ2 | TRP | A | 306 | 31.368 | 39.990 | 57.524 | 1.00 | 19.18 | AAAA |
| ATOM | 2434 | CZ3 | TRP | A | 306 | 32.474 | 41.810 | 56.367 | 1.00 | 18.98 | AAAA |
| ATOM | 2435 | CH2 | TRP | A | 306 | 31.933 | 40.513 | 56.388 | 1.00 | 19.21 | AAAA |
| ATOM | 2436 | C | TRP | A | 306 | 32.571 | 45.159 | 62.674 | 1.00 | 20.80 | AAAA |
| ATOM | 2437 | O | TRP | A | 306 | 33.459 | 44.630 | 63.341 | 1.00 | 20.55 | AAAA |
| ATOM | 2438 | N | THR | A | 307 | 32.373 | 46.475 | 62.614 | 1.00 | 20.17 | AAAA |
| ATOM | 2439 | CA | THR | A | 307 | 33.175 | 47.399 | 63.407 | 1.00 | 20.54 | AAAA |
| ATOM | 2440 | CB | THR | A | 307 | 32.861 | 48.881 | 63.045 | 1.00 | 21.09 | AAAA |
| ATOM | 2441 | OG1 | THR | A | 307 | 33.329 | 49.159 | 61.718 | 1.00 | 21.25 | AAAA |
| ATOM | 2442 | CG2 | THR | A | 307 | 33.523 | 49.839 | 64.030 | 1.00 | 20.09 | AAAA |

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Figure 19-38

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2443 | C | THR | A | 307 | 32.853 | 47.135 | 64.893 | 1.00 | 20.88 | AAAA |
| ATOM | 2444 | O | THR | A | 307 | 33.738 | 47.175 | 65.747 | 1.00 | 21.89 | AAAA |
| ATOM | 2445 | N | LEU | A | 308 | 31.588 | 46.851 | 65.192 | 1.00 | 20.10 | AAAA |
| ATOM | 2446 | CA | LEU | A | 308 | 31.189 | 46.543 | 66.559 | 1.00 | 21.10 | AAAA |
| ATOM | 2447 | CB | LEU | A | 308 | 29.671 | 46.340 | 66.644 | 1.00 | 20.99 | AAAA |
| ATOM | 2448 | CG | LEU | A | 308 | 28.897 | 47.656 | 66.674 | 1.00 | 21.54 | AAAA |
| ATOM | 2449 | CD1 | LEU | A | 308 | 27.397 | 47.473 | 66.411 | 1.00 | 19.91 | AAAA |
| ATOM | 2450 | CD2 | LEU | A | 308 | 29.177 | 48.283 | 68.045 | 1.00 | 21.04 | AAAA |
| ATOM | 2451 | C | LEU | A | 308 | 31.886 | 45.284 | 67.052 | 1.00 | 21.98 | AAAA |
| ATOM | 2452 | O | LEU | A | 308 | 32.284 | 45.186 | 68.215 | 1.00 | 22.17 | AAAA |
| ATOM | 2453 | N | ILE | A | 309 | 32.023 | 44.310 | 66.165 | 1.00 | 22.32 | AAAA |
| ATOM | 2454 | CA | ILE | A | 309 | 32.658 | 43.069 | 66.544 | 1.00 | 23.12 | AAAA |
| ATOM | 2455 | CB | ILE | A | 309 | 32.590 | 42.016 | 65.413 | 1.00 | 22.33 | AAAA |
| ATOM | 2456 | CG2 | ILE | A | 309 | 33.356 | 40.787 | 65.827 | 1.00 | 21.76 | AAAA |
| ATOM | 2457 | CG1 | ILE | A | 309 | 31.140 | 41.678 | 65.061 | 1.00 | 22.16 | AAAA |
| ATOM | 2458 | CD1 | ILE | A | 309 | 30.366 | 41.037 | 66.166 | 1.00 | 22.01 | AAAA |
| ATOM | 2459 | C | ILE | A | 309 | 34.115 | 43.377 | 66.790 | 1.00 | 24.52 | AAAA |
| ATOM | 2460 | O | ILE | A | 309 | 34.734 | 42.828 | 67.709 | 1.00 | 25.72 | AAAA |
| ATOM | 2461 | N | TRP | A | 310 | 34.673 | 44.253 | 65.957 | 1.00 | 24.70 | AAAA |
| ATOM | 2462 | CA | TRP | A | 310 | 36.075 | 44.570 | 66.099 | 1.00 | 24.20 | AAAA |
| ATOM | 2463 | CB | TRP | A | 310 | 36.587 | 45.417 | 64.944 | 1.00 | 23.29 | AAAA |
| ATOM | 2464 | CG | TRP | A | 310 | 38.040 | 45.712 | 65.123 | 1.00 | 23.17 | AAAA |
| ATOM | 2465 | CD2 | TRP | A | 310 | 39.104 | 44.752 | 65.257 | 1.00 | 21.36 | AAAA |
| ATOM | 2466 | CE2 | TRP | A | 310 | 40.291 | 45.472 | 65.490 | 1.00 | 20.62 | AAAA |
| ATOM | 2467 | CE3 | TRP | A | 310 | 39.165 | 43.354 | 65.202 | 1.00 | 20.01 | AAAA |
| ATOM | 2468 | CD1 | TRP | A | 310 | 38.614 | 46.938 | 65.273 | 1.00 | 22.82 | AAAA |
| ATOM | 2469 | NE1 | TRP | A | 310 | 39.967 | 46.803 | 65.497 | 1.00 | 22.30 | AAAA |
| ATOM | 2470 | CZ2 | TRP | A | 310 | 41.521 | 44.845 | 65.668 | 1.00 | 19.91 | AAAA |
| ATOM | 2471 | CZ3 | TRP | A | 310 | 40.388 | 42.734 | 65.381 | 1.00 | 19.08 | AAAA |
| ATOM | 2472 | CH2 | TRP | A | 310 | 41.547 | 43.477 | 65.610 | 1.00 | 19.40 | AAAA |
| ATOM | 2473 | C | TRP | A | 310 | 36.318 | 45.279 | 67.411 | 1.00 | 25.26 | AAAA |
| ATOM | 2474 | O | TRP | A | 310 | 37.262 | 44.945 | 68.109 | 1.00 | 24.71 | AAAA |
| ATOM | 2475 | N | CYS | A | 311 | 35.467 | 46.247 | 67.749 | 1.00 | 26.76 | AAAA |
| ATOM | 2476 | CA | CYS | A | 311 | 35.608 | 46.975 | 69.007 | 1.00 | 27.89 | AAAA |
| ATOM | 2477 | CB | CYS | A | 311 | 34.548 | 48.081 | 69.113 | 1.00 | 28.98 | AAAA |
| ATOM | 2478 | SG | CYS | A | 311 | 34.798 | 49.462 | 67.991 | 1.00 | 31.89 | AAAA |
| ATOM | 2479 | C | CYS | A | 311 | 35.495 | 46.043 | 70.212 | 1.00 | 27.51 | AAAA |
| ATOM | 2480 | O | CYS | A | 311 | 36.289 | 46.127 | 71.135 | 1.00 | 26.90 | AAAA |
| ATOM | 2481 | N | GLU | A | 312 | 34.495 | 45.169 | 70.187 | 1.00 | 27.33 | AAAA |
| ATOM | 2482 | CA | GLU | A | 312 | 34.246 | 44.210 | 71.250 | 1.00 | 28.03 | AAAA |
| ATOM | 2483 | CB | GLU | A | 312 | 33.106 | 43.287 | 70.850 | 1.00 | 28.55 | AAAA |
| ATOM | 2484 | CG | GLU | A | 312 | 31.903 | 43.333 | 71.741 | 1.00 | 28.93 | AAAA |
| ATOM | 2485 | CD | GLU | A | 312 | 32.232 | 42.958 | 73.154 | 1.00 | 29.78 | AAAA |
| ATOM | 2486 | OE1 | GLU | A | 312 | 32.954 | 41.957 | 73.345 | 1.00 | 30.81 | AAAA |
| ATOM | 2487 | OE2 | GLU | A | 312 | 31.754 | 43.653 | 74.071 | 1.00 | 30.79 | AAAA |
| ATOM | 2488 | C | GLU | A | 312 | 35.463 | 43.357 | 71.514 | 1.00 | 28.91 | AAAA |
| ATOM | 2489 | O | GLU | A | 312 | 35.822 | 43.110 | 72.662 | 1.00 | 30.57 | AAAA |
| ATOM | 2490 | N | LEU | A | 313 | 36.081 | 42.889 | 70.436 | 1.00 | 29.04 | AAAA |
| ATOM | 2491 | CA | LEU | A | 313 | 37.266 | 42.045 | 70.516 | 1.00 | 28.87 | AAAA |
| ATOM | 2492 | CB | LEU | A | 313 | 37.524 | 41.373 | 69.157 | 1.00 | 29.39 | AAAA |
| ATOM | 2493 | CG | LEU | A | 313 | 36.548 | 40.311 | 68.644 | 1.00 | 30.32 | AAAA |
| ATOM | 2494 | CD1 | LEU | A | 313 | 36.910 | 39.872 | 67.215 | 1.00 | 30.26 | AAAA |
| ATOM | 2495 | CD2 | LEU | A | 313 | 36.582 | 39.114 | 69.593 | 1.00 | 30.42 | AAAA |
| ATOM | 2496 | C | LEU | A | 313 | 38.474 | 42.888 | 70.905 | 1.00 | 27.75 | AAAA |
| ATOM | 2497 | O | LEU | A | 313 | 39.215 | 42.553 | 71.808 | 1.00 | 27.34 | AAAA |
| ATOM | 2498 | N | SER | A | 314 | 38.642 | 43.986 | 70.191 | 1.00 | 27.95 | AAAA |
| ATOM | 2499 | CA | SER | A | 314 | 39.736 | 44.927 | 70.376 | 1.00 | 28.62 | AAAA |
| ATOM | 2500 | CB | SER | A | 314 | 39.690 | 45.937 | 69.231 | 1.00 | 27.49 | AAAA |
| ATOM | 2501 | OG | SER | A | 314 | 40.703 | 46.904 | 69.343 | 1.00 | 30.12 | AAAA |
| ATOM | 2502 | C | SER | A | 314 | 39.666 | 45.653 | 71.727 | 1.00 | 29.67 | AAAA |
| ATOM | 2503 | O | SER | A | 314 | 40.488 | 46.517 | 72.023 | 1.00 | 29.00 | AAAA |
| ATOM | 2504 | N | GLY | A | 315 | 38.676 | 45.302 | 72.538 | 1.00 | 30.78 | AAAA |
| ATOM | 2505 | CA | GLY | A | 315 | 38.535 | 45.935 | 73.827 | 1.00 | 32.92 | AAAA |
| ATOM | 2506 | C | GLY | A | 315 | 38.542 | 47.452 | 73.784 | 1.00 | 34.92 | AAAA |
| ATOM | 2507 | O | GLY | A | 315 | 39.142 | 48.091 | 74.647 | 1.00 | 35.17 | AAAA |
| ATOM | 2508 | N | ARG | A | 316 | 37.881 | 48.041 | 72.794 | 1.00 | 36.88 | AAAA |

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Figure 19-39

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2509 | CA | ARG | A | 316 | 37.841 | 49.493 | 72.702 | 1.00 | 39.49 | AAAA |
| ATOM | 2510 | CB | ARG | A | 316 | 38.608 | 49.968 | 71.484 | 1.00 | 39.86 | AAAA |
| ATOM | 2511 | CG | ARG | A | 316 | 37.946 | 49.677 | 70.161 | 1.00 | 40.77 | AAAA |
| ATOM | 2512 | CD | ARG | A | 316 | 38.843 | 50.226 | 69.077 | 1.00 | 41.47 | AAAA |
| ATOM | 2513 | NE | ARG | A | 316 | 40.140 | 49.566 | 69.092 | 1.00 | 42.36 | AAAA |
| ATOM | 2514 | CZ | ARG | A | 316 | 41.224 | 50.057 | 68.515 | 1.00 | 43.38 | AAAA |
| ATOM | 2515 | NH1 | ARG | A | 316 | 41.159 | 51.217 | 67.882 | 1.00 | 44.76 | AAAA |
| ATOM | 2516 | NH2 | ARG | A | 316 | 42.361 | 49.385 | 68.556 | 1.00 | 43.71 | AAAA |
| ATOM | 2517 | C | ARG | A | 316 | 36.418 | 50.015 | 72.631 | 1.00 | 41.54 | AAAA |
| ATOM | 2518 | O | ARG | A | 316 | 35.564 | 49.429 | 71.959 | 1.00 | 42.64 | AAAA |
| ATOM | 2519 | N | GLU | A | 317 | 36.163 | 51.119 | 73.329 | 1.00 | 43.10 | AAAA |
| ATOM | 2520 | CA | GLU | A | 317 | 34.830 | 51.720 | 73.356 | 1.00 | 44.51 | AAAA |
| ATOM | 2521 | CB | GLU | A | 317 | 34.809 | 52.936 | 74.293 | 1.00 | 46.17 | AAAA |
| ATOM | 2522 | CG | GLU | A | 317 | 34.472 | 52.614 | 75.759 | 1.00 | 49.65 | AAAA |
| ATOM | 2523 | CD | GLU | A | 317 | 35.426 | 51.623 | 76.439 | 1.00 | 52.51 | AAAA |
| ATOM | 2524 | OE1 | GLU | A | 317 | 35.153 | 51.251 | 77.607 | 1.00 | 53.37 | AAAA |
| ATOM | 2525 | OE2 | GLU | A | 317 | 36.444 | 51.214 | 75.831 | 1.00 | 54.14 | AAAA |
| ATOM | 2526 | C | GLU | A | 317 | 34.318 | 52.098 | 71.974 | 1.00 | 43.86 | AAAA |
| ATOM | 2527 | O | GLU | A | 317 | 35.067 | 52.532 | 71.108 | 1.00 | 42.46 | AAAA |
| ATOM | 2528 | N | VAL | A | 318 | 33.023 | 51.916 | 71.779 | 1.00 | 44.79 | AAAA |
| ATOM | 2529 | CA | VAL | A | 318 | 32.394 | 52.197 | 70.502 | 1.00 | 45.57 | AAAA |
| ATOM | 2530 | CB | VAL | A | 318 | 31.098 | 51.369 | 70.324 | 1.00 | 45.36 | AAAA |
| ATOM | 2531 | CG1 | VAL | A | 318 | 30.537 | 51.558 | 68.924 | 1.00 | 45.44 | AAAA |
| ATOM | 2532 | CG2 | VAL | A | 318 | 31.366 | 49.911 | 70.612 | 1.00 | 46.35 | AAAA |
| ATOM | 2533 | C | VAL | A | 318 | 32.007 | 53.652 | 70.377 | 1.00 | 46.41 | AAAA |
| ATOM | 2534 | O | VAL | A | 318 | 31.199 | 54.145 | 71.165 | 1.00 | 46.53 | AAAA |
| ATOM | 2535 | N | PRO | A | 319 | 32.584 | 54.370 | 69.396 | 1.00 | 46.89 | AAAA |
| ATOM | 2536 | CD | PRO | A | 319 | 33.581 | 54.017 | 68.375 | 1.00 | 46.44 | AAAA |
| ATOM | 2537 | CA | PRO | A | 319 | 32.209 | 55.774 | 69.247 | 1.00 | 47.62 | AAAA |
| ATOM | 2538 | CB | PRO | A | 319 | 33.022 | 56.206 | 68.024 | 1.00 | 46.96 | AAAA |
| ATOM | 2539 | CG | PRO | A | 319 | 33.161 | 54.922 | 67.251 | 1.00 | 46.38 | AAAA |
| ATOM | 2540 | C | PRO | A | 319 | 30.709 | 55.743 | 68.977 | 1.00 | 48.64 | AAAA |
| ATOM | 2541 | O | PRO | A | 319 | 30.236 | 54.860 | 68.262 | 1.00 | 48.61 | AAAA |
| ATOM | 2542 | N | GLU | A | 320 | 29.944 | 56.667 | 69.544 | 1.00 | 49.24 | AAAA |
| ATOM | 2543 | CA | GLU | A | 320 | 28.522 | 56.598 | 69.288 | 1.00 | 50.01 | AAAA |
| ATOM | 2544 | CB | GLU | A | 320 | 27.720 | 57.330 | 70.363 | 1.00 | 51.15 | AAAA |
| ATOM | 2545 | CG | GLU | A | 320 | 27.828 | 58.831 | 70.339 | 1.00 | 53.01 | AAAA |
| ATOM | 2546 | CD | GLU | A | 320 | 26.825 | 59.474 | 71.282 | 1.00 | 54.34 | AAAA |
| ATOM | 2547 | OE1 | GLU | A | 320 | 25.604 | 59.273 | 71.077 | 1.00 | 54.04 | AAAA |
| ATOM | 2548 | OE2 | GLU | A | 320 | 27.255 | 60.171 | 72.228 | 1.00 | 55.06 | AAAA |
| ATOM | 2549 | C | GLU | A | 320 | 28.206 | 57.168 | 67.921 | 1.00 | 49.78 | AAAA |
| ATOM | 2550 | O | GLU | A | 320 | 27.170 | 56.861 | 67.324 | 1.00 | 49.79 | AAAA |
| ATOM | 2551 | N | LYS | A | 321 | 29.116 | 57.980 | 67.407 | 1.00 | 49.26 | AAAA |
| ATOM | 2552 | CA | LYS | A | 321 | 28.906 | 58.589 | 66.109 | 1.00 | 49.20 | AAAA |
| ATOM | 2553 | CB | LYS | A | 321 | 28.873 | 60.106 | 66.251 | 1.00 | 50.38 | AAAA |
| ATOM | 2554 | CG | LYS | A | 321 | 30.234 | 60.674 | 66.634 | 1.00 | 52.88 | AAAA |
| ATOM | 2555 | CD | LYS | A | 321 | 30.717 | 60.180 | 68.002 | 1.00 | 53.76 | AAAA |
| ATOM | 2556 | CE | LYS | A | 321 | 32.229 | 60.348 | 68.154 | 1.00 | 55.00 | AAAA |
| ATOM | 2557 | NZ | LYS | A | 321 | 32.715 | 61.725 | 67.829 | 1.00 | 55.95 | AAAA |
| ATOM | 2558 | C | LYS | A | 321 | 30.037 | 58.207 | 65.171 | 1.00 | 48.64 | AAAA |
| ATOM | 2559 | O | LYS | A | 321 | 31.052 | 57.650 | 65.590 | 1.00 | 48.58 | AAAA |
| ATOM | 2560 | N | LEU | A | 322 | 29.854 | 58.511 | 63.894 | 1.00 | 47.78 | AAAA |
| ATOM | 2561 | CA | LEU | A | 322 | 30.870 | 58.238 | 62.896 | 1.00 | 46.13 | AAAA |
| ATOM | 2562 | CB | LEU | A | 322 | 30.248 | 57.638 | 61.638 | 1.00 | 46.84 | AAAA |
| ATOM | 2563 | CG | LEU | A | 322 | 29.240 | 56.504 | 61.848 | 1.00 | 47.71 | AAAA |
| ATOM | 2564 | CD1 | LEU | A | 322 | 28.788 | 55.998 | 60.491 | 1.00 | 48.02 | AAAA |
| ATOM | 2565 | CD2 | LEU | A | 322 | 29.853 | 55.374 | 62.667 | 1.00 | 48.21 | AAAA |
| ATOM | 2566 | C | LEU | A | 322 | 31.427 | 59.608 | 62.580 | 1.00 | 44.61 | AAAA |
| ATOM | 2567 | O | LEU | A | 322 | 30.674 | 60.571 | 62.491 | 1.00 | 44.73 | AAAA |
| ATOM | 2568 | N | ASN | A | 323 | 32.741 | 59.706 | 62.447 | 1.00 | 42.66 | AAAA |
| ATOM | 2569 | CA | ASN | A | 323 | 33.360 | 60.976 | 62.135 | 1.00 | 41.19 | AAAA |
| ATOM | 2570 | CB | ASN | A | 323 | 34.860 | 60.904 | 62.402 | 1.00 | 41.07 | AAAA |
| ATOM | 2571 | CG | ASN | A | 323 | 35.576 | 60.001 | 61.436 | 1.00 | 41.43 | AAAA |
| ATOM | 2572 | OD1 | ASN | A | 323 | 35.117 | 58.901 | 61.147 | 1.00 | 42.46 | AAAA |
| ATOM | 2573 | ND2 | ASN | A | 323 | 36.720 | 60.449 | 60.943 | 1.00 | 41.77 | AAAA |
| ATOM | 2574 | C | ASN | A | 323 | 33.068 | 61.223 | 60.658 | 1.00 | 40.76 | AAAA |

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Figure 19-40

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|------|
| ATOM | 2575 | O | ASN A 323 | 32.430 | 60.395 | 60.010 | 1.00 | 40.19 | AAAA |
| ATOM | 2576 | N | ASN A 324 | 33.523 | 62.352 | 60.129 | 1.00 | 40.11 | AAAA |
| ATOM | 2577 | CA | ASN A 324 | 33.268 | 62.699 | 58.735 | 1.00 | 39.99 | AAAA |
| ATOM | 2578 | CB | ASN A 324 | 33.711 | 64.128 | 58.472 | 1.00 | 39.54 | AAAA |
| ATOM | 2579 | CG | ASN A 324 | 33.003 | 65.114 | 59.361 | 1.00 | 40.88 | AAAA |
| ATOM | 2580 | OD1 | ASN A 324 | 31.763 | 65.145 | 59.417 | 1.00 | 40.77 | AAAA |
| ATOM | 2581 | ND2 | ASN A 324 | 33.779 | 65.938 | 60.064 | 1.00 | 40.63 | AAAA |
| ATOM | 2582 | C | ASN A 324 | 33.918 | 61.786 | 57.712 | 1.00 | 40.10 | AAAA |
| ATOM | 2583 | O | ASN A 324 | 33.320 | 61.468 | 56.678 | 1.00 | 39.24 | AAAA |
| ATOM | 2584 | N | LYS A 325 | 35.144 | 61.376 | 58.011 | 1.00 | 40.41 | AAAA |
| ATOM | 2585 | CA | LYS A 325 | 35.908 | 60.519 | 57.126 | 1.00 | 41.41 | AAAA |
| ATOM | 2586 | CB | LYS A 325 | 37.262 | 60.201 | 57.761 | 1.00 | 42.64 | AAAA |
| ATOM | 2587 | CG | LYS A 325 | 38.224 | 59.504 | 56.828 | 1.00 | 44.45 | AAAA |
| ATOM | 2588 | CD | LYS A 325 | 39.575 | 59.199 | 57.491 | 1.00 | 45.61 | AAAA |
| ATOM | 2589 | CE | LYS A 325 | 40.358 | 60.464 | 57.850 | 1.00 | 45.88 | AAAA |
| ATOM | 2590 | NZ | LYS A 325 | 41.717 | 60.151 | 58.404 | 1.00 | 46.27 | AAAA |
| ATOM | 2591 | C | LYS A 325 | 35.124 | 59.248 | 56.856 | 1.00 | 41.56 | AAAA |
| ATOM | 2592 | O | LYS A 325 | 35.042 | 58.781 | 55.716 | 1.00 | 41.35 | AAAA |
| ATOM | 2593 | N | ALA A 326 | 34.524 | 58.703 | 57.906 | 1.00 | 41.32 | AAAA |
| ATOM | 2594 | CA | ALA A 326 | 33.732 | 57.492 | 57.774 | 1.00 | 41.07 | AAAA |
| ATOM | 2595 | CB | ALA A 326 | 33.452 | 56.912 | 59.143 | 1.00 | 40.87 | AAAA |
| ATOM | 2596 | C | ALA A 326 | 32.420 | 57.722 | 57.019 | 1.00 | 41.24 | AAAA |
| ATOM | 2597 | O | ALA A 326 | 32.045 | 56.913 | 56.174 | 1.00 | 40.91 | AAAA |
| ATOM | 2598 | N | LYS A 327 | 31.719 | 58.815 | 57.316 | 1.00 | 41.92 | AAAA |
| ATOM | 2599 | CA | LYS A 327 | 30.451 | 59.097 | 56.631 | 1.00 | 42.20 | AAAA |
| ATOM | 2600 | CB | LYS A 327 | 29.796 | 60.374 | 57.170 | 1.00 | 43.61 | AAAA |
| ATOM | 2601 | CG | LYS A 327 | 29.534 | 60.413 | 58.670 | 1.00 | 45.83 | AAAA |
| ATOM | 2602 | CD | LYS A 327 | 28.745 | 61.681 | 59.029 | 1.00 | 47.34 | AAAA |
| ATOM | 2603 | CE | LYS A 327 | 28.682 | 61.952 | 60.538 | 1.00 | 48.28 | AAAA |
| ATOM | 2604 | NZ | LYS A 327 | 28.090 | 60.845 | 61.351 | 1.00 | 48.98 | AAAA |
| ATOM | 2605 | C | LYS A 327 | 30.673 | 59.266 | 55.125 | 1.00 | 41.33 | AAAA |
| ATOM | 2606 | O | LYS A 327 | 29.879 | 58.797 | 54.309 | 1.00 | 40.78 | AAAA |
| ATOM | 2607 | N | GLU A 328 | 31.761 | 59.950 | 54.781 | 1.00 | 40.39 | AAAA |
| ATOM | 2608 | CA | GLU A 328 | 32.129 | 60.217 | 53.399 | 1.00 | 38.91 | AAAA |
| ATOM | 2609 | CB | GLU A 328 | 33.300 | 61.199 | 53.369 | 1.00 | 40.04 | AAAA |
| ATOM | 2610 | CG | GLU A 328 | 32.941 | 62.576 | 53.909 | 1.00 | 41.94 | AAAA |
| ATOM | 2611 | CD | GLU A 328 | 34.131 | 63.515 | 53.994 | 1.00 | 43.77 | AAAA |
| ATOM | 2612 | OE1 | GLU A 328 | 34.904 | 63.595 | 53.010 | 1.00 | 44.29 | AAAA |
| ATOM | 2613 | OE2 | GLU A 328 | 34.285 | 64.189 | 55.040 | 1.00 | 45.11 | AAAA |
| ATOM | 2614 | C | GLU A 328 | 32.497 | 58.938 | 52.675 | 1.00 | 37.39 | AAAA |
| ATOM | 2615 | O | GLU A 328 | 32.114 | 58.722 | 51.525 | 1.00 | 37.31 | AAAA |
| ATOM | 2616 | N | LEU A 329 | 33.255 | 58.091 | 53.355 | 1.00 | 35.67 | AAAA |
| ATOM | 2617 | CA | LEU A 329 | 33.657 | 56.820 | 52.783 | 1.00 | 33.03 | AAAA |
| ATOM | 2618 | CB | LEU A 329 | 34.451 | 56.012 | 53.813 | 1.00 | 30.62 | AAAA |
| ATOM | 2619 | CG | LEU A 329 | 34.760 | 54.549 | 53.481 | 1.00 | 27.48 | AAAA |
| ATOM | 2620 | CD1 | LEU A 329 | 35.549 | 54.453 | 52.193 | 1.00 | 26.24 | AAAA |
| ATOM | 2621 | CD2 | LEU A 329 | 35.514 | 53.936 | 54.622 | 1.00 | 25.74 | AAAA |
| ATOM | 2622 | C | LEU A 329 | 32.405 | 56.057 | 52.368 | 1.00 | 23.24 | AAAA |
| ATOM | 2623 | O | LEU A 329 | 32.239 | 55.708 | 51.205 | 1.00 | 32.72 | AAAA |
| ATOM | 2624 | N | LEU A 330 | 31.519 | 55.810 | 53.327 | 1.00 | 33.92 | AAAA |
| ATOM | 2625 | CA | LEU A 330 | 30.289 | 55.090 | 53.046 | 1.00 | 34.91 | AAAA |
| ATOM | 2626 | CB | LEU A 330 | 29.411 | 55.023 | 54.292 | 1.00 | 34.02 | AAAA |
| ATOM | 2627 | CG | LEU A 330 | 30.067 | 54.236 | 55.418 | 1.00 | 34.06 | AAAA |
| ATOM | 2628 | CD1 | LEU A 330 | 29.096 | 54.060 | 56.571 | 1.00 | 33.63 | AAAA |
| ATOM | 2629 | CD2 | LEU A 330 | 30.512 | 52.892 | 54.884 | 1.00 | 33.82 | AAAA |
| ATOM | 2630 | C | LEU A 330 | 29.499 | 55.695 | 51.907 | 1.00 | 35.94 | AAAA |
| ATOM | 2631 | O | LEU A 330 | 28.984 | 54.968 | 51.060 | 1.00 | 36.14 | AAAA |
| ATOM | 2632 | N | LYS A 331 | 29.415 | 57.022 | 51.883 | 1.00 | 38.17 | AAAA |
| ATOM | 2633 | CA | LYS A 331 | 28.664 | 57.718 | 50.845 | 1.00 | 41.05 | AAAA |
| ATOM | 2634 | CB | LYS A 331 | 28.407 | 59.161 | 51.233 | 1.00 | 41.83 | AAAA |
| ATOM | 2635 | CG | LYS A 331 | 27.584 | 59.358 | 52.497 | 1.00 | 43.26 | AAAA |
| ATOM | 2636 | CD | LYS A 331 | 27.202 | 60.823 | 52.755 | 1.00 | 44.15 | AAAA |
| ATOM | 2637 | CE | LYS A 331 | 26.182 | 61.333 | 51.730 | 1.00 | 45.71 | AAAA |
| ATOM | 2638 | NZ | LYS A 331 | 25.695 | 62.735 | 51.993 | 1.00 | 45.95 | AAAA |
| ATOM | 2639 | C | LYS A 331 | 29.342 | 57.681 | 49.490 | 1.00 | 42.22 | AAAA |
| ATOM | 2640 | O | LYS A 331 | 28.712 | 57.980 | 48.480 | 1.00 | 41.94 | AAAA |

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Figure 19-41

| | | | | | | | | | |
|------|------|-----|-----------|--------|--------|--------|------|-------|------|
| ATOM | 2641 | N | SER A 332 | 30.618 | 57.316 | 49.463 | 1.00 | 44.45 | AAAA |
| ATOM | 2642 | CA | SER A 332 | 31.351 | 57.271 | 48.202 | 1.00 | 46.88 | AAAA |
| ATOM | 2643 | CB | SER A 332 | 32.854 | 57.416 | 48.435 | 1.00 | 46.49 | AAAA |
| ATOM | 2644 | OG | SER A 332 | 33.380 | 56.263 | 49.058 | 1.00 | 45.65 | AAAA |
| ATOM | 2645 | C | SER A 332 | 31.093 | 55.959 | 47.494 | 1.00 | 48.73 | AAAA |
| ATOM | 2646 | O | SER A 332 | 31.262 | 55.854 | 46.281 | 1.00 | 49.51 | AAAA |
| ATOM | 2647 | N | ILE A 333 | 30.697 | 54.952 | 48.258 | 1.00 | 50.62 | AAAA |
| ATOM | 2648 | CA | ILE A 333 | 30.420 | 53.648 | 47.686 | 1.00 | 52.65 | AAAA |
| ATOM | 2649 | CB | ILE A 333 | 30.246 | 52.584 | 48.779 | 1.00 | 52.35 | AAAA |
| ATOM | 2650 | CG2 | ILE A 333 | 29.889 | 51.248 | 48.157 | 1.00 | 51.40 | AAAA |
| ATOM | 2651 | CG1 | ILE A 333 | 31.522 | 52.465 | 49.596 | 1.00 | 52.29 | AAAA |
| ATOM | 2652 | CD1 | ILE A 333 | 31.403 | 51.463 | 50.696 | 1.00 | 53.23 | AAAA |
| ATOM | 2653 | C | ILE A 333 | 29.120 | 53.712 | 46.924 | 1.00 | 54.42 | AAAA |
| ATOM | 2654 | O | ILE A 333 | 28.122 | 54.178 | 47.462 | 1.00 | 55.10 | AAAA |
| ATOM | 2655 | N | ASP A 334 | 29.118 | 53.274 | 45.672 | 1.00 | 56.56 | AAAA |
| ATOM | 2656 | CA | ASP A 334 | 27.863 | 53.263 | 44.940 | 1.00 | 59.13 | AAAA |
| ATOM | 2657 | CB | ASP A 334 | 28.050 | 53.460 | 43.433 | 1.00 | 59.64 | AAAA |
| ATOM | 2658 | CG | ASP A 334 | 28.976 | 52.446 | 42.823 | 1.00 | 59.23 | AAAA |
| ATOM | 2659 | OD1 | ASP A 334 | 28.853 | 52.194 | 41.606 | 1.00 | 58.87 | AAAA |
| ATOM | 2660 | OD2 | ASP A 334 | 29.839 | 51.925 | 43.559 | 1.00 | 59.34 | AAAA |
| ATOM | 2661 | C | ASP A 334 | 27.251 | 51.898 | 45.215 | 1.00 | 60.95 | AAAA |
| ATOM | 2662 | O | ASP A 334 | 27.803 | 50.861 | 44.840 | 1.00 | 61.15 | AAAA |
| ATOM | 2663 | N | PHE A 335 | 26.113 | 51.914 | 45.897 | 1.00 | 62.56 | AAAA |
| ATOM | 2664 | CA | PHE A 335 | 25.414 | 50.701 | 46.257 | 1.00 | 64.12 | AAAA |
| ATOM | 2665 | CB | PHE A 335 | 25.311 | 50.621 | 47.779 | 1.00 | 64.40 | AAAA |
| ATOM | 2666 | CG | PHE A 335 | 24.224 | 49.714 | 48.263 | 1.00 | 64.98 | AAAA |
| ATOM | 2667 | CD1 | PHE A 335 | 24.180 | 48.379 | 47.868 | 1.00 | 65.54 | AAAA |
| ATOM | 2668 | CD2 | PHE A 335 | 23.234 | 50.197 | 49.107 | 1.00 | 65.12 | AAAA |
| ATOM | 2669 | CE1 | PHE A 335 | 23.163 | 47.539 | 48.305 | 1.00 | 65.75 | AAAA |
| ATOM | 2670 | CE2 | PHE A 335 | 22.213 | 49.367 | 49.552 | 1.00 | 65.79 | AAAA |
| ATOM | 2671 | CZ | PHE A 335 | 22.177 | 48.034 | 49.150 | 1.00 | 66.01 | AAAA |
| ATOM | 2672 | C | PHE A 335 | 24.025 | 50.626 | 45.640 | 1.00 | 65.41 | AAAA |
| ATOM | 2673 | O | PHE A 335 | 23.591 | 49.564 | 45.184 | 1.00 | 65.27 | AAAA |
| ATOM | 2674 | N | GLU A 336 | 23.338 | 51.763 | 45.618 | 1.00 | 66.38 | AAAA |
| ATOM | 2675 | CA | GLU A 336 | 21.980 | 51.826 | 45.097 | 1.00 | 67.49 | AAAA |
| ATOM | 2676 | CB | GLU A 336 | 21.893 | 51.260 | 43.673 | 1.00 | 68.25 | AAAA |
| ATOM | 2677 | CG | GLU A 336 | 20.459 | 51.230 | 43.116 | 1.00 | 69.15 | AAAA |
| ATOM | 2678 | CD | GLU A 336 | 20.334 | 50.465 | 41.804 | 1.00 | 69.40 | AAAA |
| ATOM | 2679 | OE1 | GLU A 336 | 20.710 | 49.271 | 41.784 | 1.00 | 69.57 | AAAA |
| ATOM | 2680 | OE2 | GLU A 336 | 19.851 | 51.051 | 40.804 | 1.00 | 69.10 | AAAA |
| ATOM | 2681 | C | GLU A 336 | 21.098 | 50.999 | 46.025 | 1.00 | 67.68 | AAAA |
| ATOM | 2682 | O | GLU A 336 | 21.216 | 49.776 | 46.082 | 1.00 | 67.58 | AAAA |
| ATOM | 2683 | N | GLU A 337 | 20.227 | 51.679 | 46.761 | 1.00 | 67.87 | AAAA |
| ATOM | 2684 | CA | GLU A 337 | 19.317 | 51.020 | 47.686 | 1.00 | 68.66 | AAAA |
| ATOM | 2685 | CB | GLU A 337 | 18.583 | 52.085 | 48.502 | 1.00 | 68.88 | AAAA |
| ATOM | 2686 | CG | GLU A 337 | 18.279 | 51.715 | 49.944 | 1.00 | 68.12 | AAAA |
| ATOM | 2687 | CD | GLU A 337 | 19.527 | 51.587 | 50.789 | 1.00 | 67.70 | AAAA |
| ATOM | 2688 | OE1 | GLU A 337 | 20.319 | 52.554 | 50.851 | 1.00 | 67.05 | AAAA |
| ATOM | 2689 | OE2 | GLU A 337 | 19.711 | 50.518 | 51.398 | 1.00 | 67.79 | AAAA |
| ATOM | 2690 | C | GLU A 337 | 18.322 | 50.222 | 46.827 | 1.00 | 69.28 | AAAA |
| ATOM | 2691 | O | GLU A 337 | 17.886 | 50.705 | 45.780 | 1.00 | 69.50 | AAAA |
| ATOM | 2692 | N | PHE A 338 | 17.966 | 49.012 | 47.259 | 1.00 | 69.55 | AAAA |
| ATOM | 2693 | CA | PHE A 338 | 17.035 | 48.176 | 46.497 | 1.00 | 69.67 | AAAA |
| ATOM | 2694 | CB | PHE A 338 | 16.995 | 46.759 | 47.066 | 1.00 | 70.51 | AAAA |
| ATOM | 2695 | CG | PHE A 338 | 16.225 | 45.789 | 46.221 | 1.00 | 71.57 | AAAA |
| ATOM | 2696 | CD1 | PHE A 338 | 16.666 | 45.462 | 44.936 | 1.00 | 72.04 | AAAA |
| ATOM | 2697 | CD2 | PHE A 338 | 15.052 | 45.208 | 46.698 | 1.00 | 71.69 | AAAA |
| ATOM | 2698 | CE1 | PHE A 338 | 15.944 | 44.566 | 44.138 | 1.00 | 72.23 | AAAA |
| ATOM | 2699 | CE2 | PHE A 338 | 14.323 | 44.313 | 45.909 | 1.00 | 71.93 | AAAA |
| ATOM | 2700 | CZ | PHE A 338 | 14.770 | 43.991 | 44.627 | 1.00 | 72.11 | AAAA |
| ATOM | 2701 | C | PHE A 338 | 15.633 | 48.770 | 46.494 | 1.00 | 69.26 | AAAA |
| ATOM | 2702 | O | PHE A 338 | 15.072 | 49.029 | 45.434 | 1.00 | 68.86 | AAAA |
| ATOM | 2703 | N | ASP A 339 | 15.053 | 48.962 | 47.674 | 1.00 | 69.35 | AAAA |
| ATOM | 2704 | CA | ASP A 339 | 13.733 | 49.572 | 47.755 | 1.00 | 69.61 | AAAA |
| ATOM | 2705 | CB | ASP A 339 | 13.134 | 49.457 | 49.157 | 1.00 | 69.48 | AAAA |
| ATOM | 2706 | CG | ASP A 339 | 11.819 | 50.233 | 49.299 | 1.00 | 69.72 | AAAA |

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Figure 19-42

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2707 | OD1 | ASP | A | 339 | 11.813 | 51.462 | 49.058 | 1.00 | 69.39 | AAAA |
| ATOM | 2708 | OD2 | ASP | A | 339 | 10.790 | 49.618 | 49.655 | 1.00 | 69.78 | AAAA |
| ATOM | 2709 | C | ASP | A | 339 | 13.972 | 51.035 | 47.440 | 1.00 | 69.95 | AAAA |
| ATOM | 2710 | O | ASP | A | 339 | 14.305 | 51.815 | 48.333 | 1.00 | 69.92 | AAAA |
| ATOM | 2711 | N | ASP | A | 340 | 13.810 | 51.389 | 46.168 | 1.00 | 70.23 | AAAA |
| ATOM | 2712 | CA | ASP | A | 340 | 14.023 | 52.748 | 45.699 | 1.00 | 70.39 | AAAA |
| ATOM | 2713 | CB | ASP | A | 340 | 12.757 | 53.283 | 45.041 | 1.00 | 70.64 | AAAA |
| ATOM | 2714 | CG | ASP | A | 340 | 12.397 | 52.517 | 43.791 | 1.00 | 70.86 | AAAA |
| ATOM | 2715 | OD1 | ASP | A | 340 | 12.126 | 51.302 | 43.903 | 1.00 | 70.93 | AAAA |
| ATOM | 2716 | OD2 | ASP | A | 340 | 12.399 | 53.125 | 42.699 | 1.00 | 70.89 | AAAA |
| ATOM | 2717 | C | ASP | A | 340 | 14.482 | 53.674 | 46.807 | 1.00 | 70.63 | AAAA |
| ATOM | 2718 | O | ASP | A | 340 | 15.688 | 53.847 | 47.008 | 1.00 | 71.13 | AAAA |
| ATOM | 2719 | N | GLU | A | 341 | 13.543 | 54.259 | 47.544 | 1.00 | 69.95 | AAAA |
| ATOM | 2720 | CA | GLU | A | 341 | 13.947 | 55.150 | 48.619 | 1.00 | 69.17 | AAAA |
| ATOM | 2721 | CB | GLU | A | 341 | 13.636 | 56.613 | 48.266 | 1.00 | 70.83 | AAAA |
| ATOM | 2722 | CG | GLU | A | 341 | 14.098 | 57.601 | 49.347 | 1.00 | 73.44 | AAAA |
| ATOM | 2723 | CD | GLU | A | 341 | 13.956 | 59.071 | 48.951 | 1.00 | 75.27 | AAAA |
| ATOM | 2724 | OE1 | GLU | A | 341 | 12.825 | 59.518 | 48.646 | 1.00 | 76.21 | AAAA |
| ATOM | 2725 | OE2 | GLU | A | 341 | 14.984 | 59.786 | 48.954 | 1.00 | 75.69 | AAAA |
| ATOM | 2726 | C | GLU | A | 341 | 13.367 | 54.819 | 49.983 | 1.00 | 67.09 | AAAA |
| ATOM | 2727 | O | GLU | A | 341 | 12.233 | 55.176 | 50.297 | 1.00 | 66.57 | AAAA |
| ATOM | 2728 | N | VAL | A | 342 | 14.158 | 54.114 | 50.785 | 1.00 | 64.87 | AAAA |
| ATOM | 2729 | CA | VAL | A | 342 | 13.767 | 53.779 | 52.148 | 1.00 | 62.55 | AAAA |
| ATOM | 2730 | CB | VAL | A | 342 | 14.265 | 52.377 | 52.589 | 1.00 | 62.81 | AAAA |
| ATOM | 2731 | CG1 | VAL | A | 342 | 14.042 | 52.193 | 54.081 | 1.00 | 62.56 | AAAA |
| ATOM | 2732 | CG2 | VAL | A | 342 | 13.513 | 51.298 | 51.849 | 1.00 | 63.69 | AAAA |
| ATOM | 2733 | C | VAL | A | 342 | 14.483 | 54.822 | 52.982 | 1.00 | 59.94 | AAAA |
| ATOM | 2734 | O | VAL | A | 342 | 14.022 | 55.215 | 54.054 | 1.00 | 59.91 | AAAA |
| ATOM | 2735 | N | ASP | A | 343 | 15.609 | 55.278 | 52.442 | 1.00 | 56.85 | AAAA |
| ATOM | 2736 | CA | ASP | A | 343 | 16.457 | 56.266 | 53.085 | 1.00 | 54.01 | AAAA |
| ATOM | 2737 | CB | ASP | A | 343 | 15.639 | 57.446 | 53.605 | 1.00 | 54.18 | AAAA |
| ATOM | 2738 | CG | ASP | A | 343 | 16.505 | 58.511 | 54.241 | 1.00 | 53.96 | AAAA |
| ATOM | 2739 | OD1 | ASP | A | 343 | 15.947 | 59.485 | 54.785 | 1.00 | 54.59 | AAAA |
| ATOM | 2740 | OD2 | ASP | A | 343 | 17.747 | 58.373 | 54.191 | 1.00 | 53.61 | AAAA |
| ATOM | 2741 | C | ASP | A | 343 | 17.186 | 55.609 | 54.242 | 1.00 | 51.92 | AAAA |
| ATOM | 2742 | O | ASP | A | 343 | 16.611 | 55.371 | 55.307 | 1.00 | 51.89 | AAAA |
| ATOM | 2743 | N | ARG | A | 344 | 18.458 | 55.306 | 54.029 | 1.00 | 48.86 | AAAA |
| ATOM | 2744 | CA | ARG | A | 344 | 19.240 | 54.676 | 55.069 | 1.00 | 45.59 | AAAA |
| ATOM | 2745 | CB | ARG | A | 344 | 19.847 | 53.369 | 54.573 | 1.00 | 43.94 | AAAA |
| ATOM | 2746 | CG | ARG | A | 344 | 18.847 | 52.289 | 54.220 | 1.00 | 41.70 | AAAA |
| ATOM | 2747 | CD | ARG | A | 344 | 17.953 | 51.955 | 55.385 | 1.00 | 38.94 | AAAA |
| ATOM | 2748 | NE | ARG | A | 344 | 17.139 | 50.781 | 55.096 | 1.00 | 36.78 | AAAA |
| ATOM | 2749 | CZ | ARG | A | 344 | 16.176 | 50.316 | 55.888 | 1.00 | 34.81 | AAAA |
| ATOM | 2750 | NH1 | ARG | A | 344 | 15.890 | 50.927 | 57.033 | 1.00 | 34.11 | AAAA |
| ATOM | 2751 | NH2 | ARG | A | 344 | 15.506 | 49.228 | 55.537 | 1.00 | 31.84 | AAAA |
| ATOM | 2752 | C | ARG | A | 344 | 20.340 | 55.604 | 55.520 | 1.00 | 44.83 | AAAA |
| ATOM | 2753 | O | ARG | A | 344 | 21.308 | 55.157 | 56.128 | 1.00 | 43.97 | AAAA |
| ATOM | 2754 | N | SER | A | 345 | 20.192 | 56.895 | 55.226 | 1.00 | 44.32 | AAAA |
| ATOM | 2755 | CA | SER | A | 345 | 21.199 | 57.877 | 55.618 | 1.00 | 43.74 | AAAA |
| ATOM | 2756 | CB | SER | A | 345 | 20.860 | 59.248 | 55.039 | 1.00 | 44.49 | AAAA |
| ATOM | 2757 | OG | SER | A | 345 | 19.645 | 59.729 | 55.577 | 1.00 | 46.07 | AAAA |
| ATOM | 2758 | C | SER | A | 345 | 21.307 | 57.977 | 57.144 | 1.00 | 42.82 | AAAA |
| ATOM | 2759 | O | SER | A | 345 | 22.304 | 58.472 | 57.674 | 1.00 | 42.91 | AAAA |
| ATOM | 2760 | N | TYR | A | 346 | 20.282 | 57.509 | 57.849 | 1.00 | 41.48 | AAAA |
| ATOM | 2761 | CA | TYR | A | 346 | 20.296 | 57.549 | 59.303 | 1.00 | 40.35 | AAAA |
| ATOM | 2762 | CB | TYR | A | 346 | 18.947 | 57.068 | 59.858 | 1.00 | 40.38 | AAAA |
| ATOM | 2763 | CG | TYR | A | 346 | 18.630 | 55.601 | 59.609 | 1.00 | 39.28 | AAAA |
| ATOM | 2764 | CD1 | TYR | A | 346 | 19.293 | 54.589 | 60.316 | 1.00 | 38.74 | AAAA |
| ATOM | 2765 | CE1 | TYR | A | 346 | 19.022 | 53.243 | 60.079 | 1.00 | 37.71 | AAAA |
| ATOM | 2766 | CD2 | TYR | A | 346 | 17.682 | 55.225 | 58.653 | 1.00 | 38.49 | AAAA |
| ATOM | 2767 | CE2 | TYR | A | 346 | 17.405 | 53.882 | 58.408 | 1.00 | 38.17 | AAAA |
| ATOM | 2768 | CZ | TYR | A | 346 | 18.079 | 52.899 | 59.126 | 1.00 | 37.59 | AAAA |
| ATOM | 2769 | OH | TYR | A | 346 | 17.794 | 51.580 | 58.898 | 1.00 | 37.14 | AAAA |
| ATOM | 2770 | C | TYR | A | 346 | 21.436 | 56.686 | 59.849 | 1.00 | 39.91 | AAAA |
| ATOM | 2771 | O | TYR | A | 346 | 21.967 | 56.957 | 60.921 | 1.00 | 40.28 | AAAA |
| ATOM | 2772 | N | MET | A | 347 | 21.800 | 55.640 | 59.113 | 1.00 | 39.14 | AAAA |

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Figure 19-43

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2773 | CA | MET | A | 347 | 22.879 | 54.756 | 59.530 | 1.00 | 38.19 | AAAA |
| ATOM | 2774 | CB | MET | A | 347 | 23.042 | 53.582 | 58.566 | 1.00 | 38.26 | AAAA |
| ATOM | 2775 | CG | MET | A | 347 | 21.973 | 52.523 | 58.694 | 1.00 | 38.17 | AAAA |
| ATOM | 2776 | SD | MET | A | 347 | 22.317 | 51.115 | 57.641 | 1.00 | 38.05 | AAAA |
| ATOM | 2777 | CE | MET | A | 347 | 22.237 | 51.892 | 56.101 | 1.00 | 37.61 | AAAA |
| ATOM | 2778 | C | MET | A | 347 | 24.189 | 55.494 | 59.603 | 1.00 | 38.00 | AAAA |
| ATOM | 2779 | O | MET | A | 347 | 25.127 | 55.033 | 60.250 | 1.00 | 37.40 | AAAA |
| ATOM | 2780 | N | LEU | A | 348 | 24.248 | 56.637 | 58.929 | 1.00 | 38.08 | AAAA |
| ATOM | 2781 | CA | LEU | A | 348 | 25.449 | 57.463 | 58.898 | 1.00 | 38.07 | AAAA |
| ATOM | 2782 | CB | LEU | A | 348 | 25.445 | 58.330 | 57.638 | 1.00 | 36.66 | AAAA |
| ATOM | 2783 | CG | LEU | A | 348 | 25.379 | 57.583 | 56.310 | 1.00 | 35.47 | AAAA |
| ATOM | 2784 | CD1 | LEU | A | 348 | 25.285 | 58.559 | 55.165 | 1.00 | 34.51 | AAAA |
| ATOM | 2785 | CD2 | LEU | A | 348 | 26.605 | 56.716 | 56.167 | 1.00 | 36.56 | AAAA |
| ATOM | 2786 | C | LEU | A | 348 | 25.521 | 58.353 | 60.138 | 1.00 | 39.07 | AAAA |
| ATOM | 2787 | O | LEU | A | 348 | 26.546 | 58.980 | 60.406 | 1.00 | 38.81 | AAAA |
| ATOM | 2788 | N | GLU | A | 349 | 24.432 | 58.385 | 60.898 | 1.00 | 39.90 | AAAA |
| ATOM | 2789 | CA | GLU | A | 349 | 24.363 | 59.213 | 62.092 | 1.00 | 40.95 | AAAA |
| ATOM | 2790 | CB | GLU | A | 349 | 22.961 | 59.821 | 62.203 | 1.00 | 41.70 | AAAA |
| ATOM | 2791 | CG | GLU | A | 349 | 22.515 | 60.629 | 60.966 | 1.00 | 42.28 | AAAA |
| ATOM | 2792 | CD | GLU | A | 349 | 23.349 | 61.891 | 60.708 | 1.00 | 42.51 | AAAA |
| ATOM | 2793 | OE1 | GLU | A | 349 | 23.414 | 62.778 | 61.587 | 1.00 | 42.38 | AAAA |
| ATOM | 2794 | OE2 | GLU | A | 349 | 23.933 | 61.998 | 59.614 | 1.00 | 43.34 | AAAA |
| ATOM | 2795 | C | GLU | A | 349 | 24.740 | 58.511 | 63.406 | 1.00 | 41.12 | AAAA |
| ATOM | 2796 | O | GLU | A | 349 | 24.664 | 59.118 | 64.476 | 1.00 | 41.38 | AAAA |
| ATOM | 2797 | N | THR | A | 350 | 25.140 | 57.243 | 63.326 | 1.00 | 40.86 | AAAA |
| ATOM | 2798 | CA | THR | A | 350 | 25.555 | 56.475 | 64.504 | 1.00 | 40.69 | AAAA |
| ATOM | 2799 | CB | THR | A | 350 | 24.405 | 56.283 | 65.510 | 1.00 | 41.56 | AAAA |
| ATOM | 2800 | OG1 | THR | A | 350 | 24.062 | 57.549 | 66.078 | 1.00 | 41.48 | AAAA |
| ATOM | 2801 | CG2 | THR | A | 350 | 24.821 | 55.345 | 66.638 | 1.00 | 41.19 | AAAA |
| ATOM | 2802 | C | THR | A | 350 | 26.109 | 55.109 | 64.141 | 1.00 | 40.14 | AAAA |
| ATOM | 2803 | O | THR | A | 350 | 25.857 | 54.595 | 63.055 | 1.00 | 39.93 | AAAA |
| ATOM | 2804 | N | LEU | A | 351 | 26.865 | 54.527 | 65.067 | 1.00 | 40.32 | AAAA |
| ATOM | 2805 | CA | LEU | A | 351 | 27.491 | 53.227 | 64.857 | 1.00 | 40.70 | AAAA |
| ATOM | 2806 | CB | LEU | A | 351 | 28.855 | 53.213 | 65.540 | 1.00 | 39.89 | AAAA |
| ATOM | 2807 | CG | LEU | A | 351 | 29.911 | 52.290 | 64.951 | 1.00 | 39.68 | AAAA |
| ATOM | 2808 | CD1 | LEU | A | 351 | 31.170 | 52.403 | 65.772 | 1.00 | 39.88 | AAAA |
| ATOM | 2809 | CD2 | LEU | A | 351 | 29.414 | 50.861 | 64.945 | 1.00 | 40.70 | AAAA |
| ATOM | 2810 | C | LEU | A | 351 | 26.612 | 52.091 | 65.384 | 1.00 | 41.12 | AAAA |
| ATOM | 2811 | O | LEU | A | 351 | 26.467 | 51.060 | 64.736 | 1.00 | 40.02 | AAAA |
| ATOM | 2812 | N | LYS | A | 352 | 26.040 | 52.292 | 66.567 | 1.00 | 42.99 | AAAA |
| ATOM | 2813 | CA | LYS | A | 352 | 25.138 | 51.326 | 67.201 | 1.00 | 43.93 | AAAA |
| ATOM | 2814 | CB | LYS | A | 352 | 25.412 | 51.225 | 68.707 | 1.00 | 43.38 | AAAA |
| ATOM | 2815 | CG | LYS | A | 352 | 26.743 | 50.597 | 69.055 | 1.00 | 44.68 | AAAA |
| ATOM | 2816 | CD | LYS | A | 352 | 27.185 | 50.927 | 70.482 | 1.00 | 45.48 | AAAA |
| ATOM | 2817 | CE | LYS | A | 352 | 26.189 | 50.500 | 71.539 | 1.00 | 46.21 | AAAA |
| ATOM | 2818 | NZ | LYS | A | 352 | 26.646 | 50.944 | 72.895 | 1.00 | 47.34 | AAAA |
| ATOM | 2819 | C | LYS | A | 352 | 23.723 | 51.838 | 67.003 | 1.00 | 44.40 | AAAA |
| ATOM | 2820 | O | LYS | A | 352 | 23.375 | 52.917 | 67.488 | 1.00 | 45.79 | AAAA |
| ATOM | 2821 | N | ASP | A | 353 | 22.904 | 51.083 | 66.287 | 1.00 | 44.78 | AAAA |
| ATOM | 2822 | CA | ASP | A | 353 | 21.532 | 51.509 | 66.074 | 1.00 | 44.79 | AAAA |
| ATOM | 2823 | CB | ASP | A | 353 | 21.050 | 51.030 | 64.702 | 1.00 | 45.20 | AAAA |
| ATOM | 2824 | CG | ASP | A | 353 | 21.146 | 49.544 | 64.546 | 1.00 | 45.21 | AAAA |
| ATOM | 2825 | OD1 | ASP | A | 353 | 21.806 | 49.086 | 63.581 | 1.00 | 45.06 | AAAA |
| ATOM | 2826 | OD2 | ASP | A | 353 | 20.549 | 48.841 | 65.391 | 1.00 | 45.54 | AAAA |
| ATOM | 2827 | C | ASP | A | 353 | 20.645 | 50.993 | 67.217 | 1.00 | 44.44 | AAAA |
| ATOM | 2828 | O | ASP | A | 353 | 21.042 | 50.113 | 67.973 | 1.00 | 44.29 | AAAA |
| ATOM | 2829 | N | PRO | A | 354 | 19.439 | 51.553 | 67.367 | 1.00 | 44.22 | AAAA |
| ATOM | 2830 | CD | PRO | A | 354 | 18.839 | 52.617 | 66.550 | 1.00 | 44.38 | AAAA |
| ATOM | 2831 | CA | PRO | A | 354 | 18.500 | 51.163 | 68.419 | 1.00 | 44.18 | AAAA |
| ATOM | 2832 | CB | PRO | A | 354 | 17.371 | 52.170 | 68.238 | 1.00 | 44.52 | AAAA |
| ATOM | 2833 | CG | PRO | A | 354 | 17.368 | 52.341 | 66.749 | 1.00 | 44.66 | AAAA |
| ATOM | 2834 | C | PRO | A | 354 | 17.995 | 49.740 | 68.328 | 1.00 | 43.87 | AAAA |
| ATOM | 2835 | O | PRO | A | 354 | 17.962 | 49.152 | 67.249 | 1.00 | 44.48 | AAAA |
| ATOM | 2836 | N | TRP | A | 355 | 17.588 | 49.198 | 69.469 | 1.00 | 43.23 | AAAA |
| ATOM | 2837 | CA | TRP | A | 355 | 17.051 | 47.851 | 69.500 | 1.00 | 42.88 | AAAA |
| ATOM | 2838 | CB | TRP | A | 355 | 16.743 | 47.401 | 70.927 | 1.00 | 46.42 | AAAA |

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Figure 19-44

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2839 | CG | TRP | A | 355 | 17.959 | 47.052 | 71.695 | 1.00 | 49.91 | AAAA |
| ATOM | 2840 | CD2 | TBP | A | 355 | 18.476 | 45.733 | 71.903 | 1.00 | 51.56 | AAAA |
| ATOM | 2841 | CE2 | TRP | A | 355 | 19.684 | 45.868 | 72.627 | 1.00 | 52.03 | AAAA |
| ATOM | 2842 | CE3 | TRP | A | 355 | 18.038 | 44.450 | 71.548 | 1.00 | 52.25 | AAAA |
| ATOM | 2843 | CD1 | TRP | A | 355 | 18.846 | 47.915 | 72.284 | 1.00 | 50.53 | AAAA |
| ATOM | 2844 | NE1 | TRP | A | 355 | 19.885 | 47.208 | 72.846 | 1.00 | 51.63 | AAAA |
| ATOM | 2845 | CZ2 | TRP | A | 355 | 20.460 | 44.763 | 73.003 | 1.00 | 52.64 | AAAA |
| ATOM | 2846 | CZ3 | TRP | A | 355 | 18.810 | 43.352 | 71.921 | 1.00 | 53.12 | AAAA |
| ATOM | 2847 | CH2 | TRP | A | 355 | 20.008 | 43.518 | 72.642 | 1.00 | 53.02 | AAAA |
| ATOM | 2848 | C | TRP | A | 355 | 15.788 | 47.767 | 68.675 | 1.00 | 40.28 | AAAA |
| ATOM | 2849 | O | TRP | A | 355 | 15.017 | 48.720 | 68.591 | 1.00 | 39.82 | AAAA |
| ATOM | 2850 | N | ARG | A | 356 | 15.591 | 46.610 | 68.065 | 1.00 | 36.83 | AAAA |
| ATOM | 2851 | CA | ARG | A | 356 | 14.440 | 46.365 | 67.225 | 1.00 | 33.70 | AAAA |
| ATOM | 2852 | CB | ARG | A | 356 | 14.901 | 46.197 | 65.772 | 1.00 | 29.50 | AAAA |
| ATOM | 2853 | CG | ARG | A | 356 | 15.635 | 47.423 | 65.256 | 1.00 | 25.22 | AAAA |
| ATOM | 2854 | CD | ARG | A | 356 | 16.418 | 47.194 | 63.973 | 1.00 | 21.53 | AAAA |
| ATOM | 2855 | NE | ARG | A | 356 | 17.055 | 48.435 | 63.533 | 1.00 | 18.55 | AAAA |
| ATOM | 2856 | CZ | ARG | A | 356 | 17.976 | 48.533 | 62.574 | 1.00 | 17.06 | AAAA |
| ATOM | 2857 | NH1 | ARG | A | 356 | 18.403 | 47.451 | 61.919 | 1.00 | 17.64 | AAAA |
| ATOM | 2858 | NH2 | ARG | A | 356 | 18.445 | 49.721 | 62.241 | 1.00 | 11.56 | AAAA |
| ATOM | 2859 | C | ARG | A | 356 | 13.831 | 45.095 | 67.773 | 1.00 | 34.63 | AAAA |
| ATOM | 2860 | O | ARG | A | 356 | 13.605 | 44.117 | 67.051 | 1.00 | 35.86 | AAAA |
| ATOM | 2861 | N | GLY | A | 357 | 13.587 | 45.112 | 69.079 | 1.00 | 34.58 | AAAA |
| ATOM | 2862 | CA | GLY | A | 357 | 13.003 | 43.960 | 69.734 | 1.00 | 34.33 | AAAA |
| ATOM | 2863 | C | GLY | A | 357 | 11.536 | 43.783 | 69.395 | 1.00 | 34.31 | AAAA |
| ATOM | 2864 | O | GLY | A | 357 | 11.006 | 44.418 | 68.484 | 1.00 | 33.56 | AAAA |
| ATOM | 2865 | N | GLY | A | 358 | 10.876 | 42.906 | 70.139 | 1.00 | 34.47 | AAAA |
| ATOM | 2866 | CA | GLY | A | 358 | 9.468 | 42.656 | 69.916 | 1.00 | 34.61 | AAAA |
| ATOM | 2867 | C | GLY | A | 358 | 9.114 | 41.389 | 70.655 | 1.00 | 34.47 | AAAA |
| ATOM | 2868 | O | GLY | A | 358 | 9.962 | 40.821 | 71.345 | 1.00 | 34.27 | AAAA |
| ATOM | 2869 | N | GLU | A | 359 | 7.869 | 40.948 | 70.523 | 1.00 | 34.16 | AAAA |
| ATOM | 2870 | CA | GLU | A | 359 | 7.438 | 39.729 | 71.180 | 1.00 | 33.94 | AAAA |
| ATOM | 2871 | CB | GLU | A | 359 | 5.910 | 39.644 | 71.174 | 1.00 | 34.78 | AAAA |
| ATOM | 2872 | CG | GLU | A | 359 | 5.278 | 40.648 | 72.123 | 1.00 | 36.70 | AAAA |
| ATOM | 2873 | CD | GLU | A | 359 | 3.863 | 41.020 | 71.740 | 1.00 | 38.40 | AAAA |
| ATOM | 2874 | OE1 | GLU | A | 359 | 3.017 | 40.108 | 71.600 | 1.00 | 39.65 | AAAA |
| ATOM | 2875 | OE2 | GLU | A | 359 | 3.598 | 42.234 | 71.584 | 1.00 | 38.52 | AAAA |
| ATOM | 2876 | C | GLU | A | 359 | 8.058 | 38.549 | 70.464 | 1.00 | 32.86 | AAAA |
| ATOM | 2877 | O | GLU | A | 359 | 8.678 | 38.692 | 69.427 | 1.00 | 32.92 | AAAA |
| ATOM | 2878 | N | VAL | A | 360 | 7.918 | 37.375 | 71.036 | 1.00 | 32.63 | AAAA |
| ATOM | 2879 | CA | VAL | A | 360 | 8.480 | 36.215 | 70.409 | 1.00 | 32.70 | AAAA |
| ATOM | 2880 | CB | VAL | A | 360 | 9.422 | 35.472 | 71.376 | 1.00 | 33.24 | AAAA |
| ATOM | 2881 | CG1 | VAL | A | 360 | 10.017 | 34.252 | 70.701 | 1.00 | 32.99 | AAAA |
| ATOM | 2882 | CG2 | VAL | A | 360 | 10.521 | 36.406 | 71.827 | 1.00 | 32.09 | AAAA |
| ATOM | 2883 | C | VAL | A | 360 | 7.339 | 35.319 | 69.976 | 1.00 | 32.81 | AAAA |
| ATOM | 2884 | O | VAL | A | 360 | 6.702 | 34.660 | 70.791 | 1.00 | 32.02 | AAAA |
| ATOM | 2885 | N | ARG | A | 361 | 7.084 | 35.321 | 68.674 | 1.00 | 33.12 | AAAA |
| ATOM | 2886 | CA | ARG | A | 361 | 6.035 | 34.508 | 68.086 | 1.00 | 33.52 | AAAA |
| ATOM | 2887 | CB | ARG | A | 361 | 6.148 | 34.558 | 66.565 | 1.00 | 33.43 | AAAA |
| ATOM | 2888 | CG | ARG | A | 361 | 5.731 | 35.885 | 65.967 | 1.00 | 34.35 | AAAA |
| ATOM | 2889 | CD | ARG | A | 361 | 6.041 | 35.972 | 64.469 | 1.00 | 33.90 | AAAA |
| ATOM | 2890 | NE | ARG | A | 361 | 7.430 | 36.331 | 64.193 | 1.00 | 31.70 | AAAA |
| ATOM | 2891 | CZ | ARG | A | 361 | 7.890 | 36.608 | 62.978 | 1.00 | 31.18 | AAAA |
| ATOM | 2892 | NH1 | ARG | A | 361 | 7.068 | 36.562 | 61.941 | 1.00 | 30.48 | AAAA |
| ATOM | 2893 | NH2 | ARG | A | 361 | 9.162 | 36.948 | 62.802 | 1.00 | 29.71 | AAAA |
| ATOM | 2894 | C | ARG | A | 361 | 6.066 | 33.057 | 68.557 | 1.00 | 34.20 | AAAA |
| ATOM | 2895 | O | ARG | A | 361 | 7.101 | 32.537 | 68.968 | 1.00 | 33.79 | AAAA |
| ATOM | 2896 | N | LYS | A | 362 | 4.914 | 32.407 | 68.496 | 1.00 | 34.68 | AAAA |
| ATOM | 2897 | CA | LYS | A | 362 | 4.808 | 31.022 | 68.901 | 1.00 | 35.62 | AAAA |
| ATOM | 2898 | CB | LYS | A | 362 | 3.350 | 30.555 | 68.782 | 1.00 | 37.80 | AAAA |
| ATOM | 2899 | CG | LYS | A | 362 | 2.378 | 31.226 | 69.756 | 1.00 | 40.38 | AAAA |
| ATOM | 2900 | CD | LYS | A | 362 | 2.505 | 32.777 | 69.777 | 1.00 | 42.09 | AAAA |
| ATOM | 2901 | CE | LYS | A | 362 | 2.208 | 33.446 | 68.420 | 1.00 | 41.94 | AAAA |
| ATOM | 2902 | NZ | LYS | A | 362 | 2.473 | 34.909 | 68.451 | 1.00 | 39.85 | AAAA |
| ATOM | 2903 | C | LYS | A | 362 | 5.710 | 30.177 | 68.005 | 1.00 | 35.12 | AAAA |
| ATOM | 2904 | O | LYS | A | 362 | 6.425 | 29.301 | 68.487 | 1.00 | 34.14 | AAAA |

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Figure 19-45

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2905 | N | GLU | A | 363 | 5.661 | 30.460 | 66.703 | 1.00 | 35.12 | AAAA |
| ATOM | 2906 | CA | GLU | A | 363 | 6.445 | 29.741 | 65.699 | 1.00 | 35.62 | AAAA |
| ATOM | 2907 | CB | GLU | A | 363 | 6.567 | 30.560 | 64.424 | 1.00 | 36.81 | AAAA |
| ATOM | 2908 | CG | GLU | A | 363 | 5.280 | 30.808 | 63.711 | 1.00 | 38.66 | AAAA |
| ATOM | 2909 | CD | GLU | A | 363 | 5.477 | 31.704 | 62.517 | 1.00 | 39.60 | AAAA |
| ATOM | 2910 | OE1 | GLU | A | 363 | 6.287 | 31.324 | 61.637 | 1.00 | 39.11 | AAAA |
| ATOM | 2911 | OE2 | GLU | A | 363 | 4.826 | 32.782 | 62.469 | 1.00 | 39.95 | AAAA |
| ATOM | 2912 | C | GLU | A | 363 | 7.836 | 29.450 | 66.181 | 1.00 | 35.14 | AAAA |
| ATOM | 2913 | O | GLU | A | 363 | 8.321 | 28.316 | 66.098 | 1.00 | 34.50 | AAAA |
| ATOM | 2914 | N | VAL | A | 364 | 8.475 | 30.505 | 66.671 | 1.00 | 34.96 | AAAA |
| ATOM | 2915 | CA | VAL | A | 364 | 9.830 | 30.431 | 67.180 | 1.00 | 34.44 | AAAA |
| ATOM | 2916 | CB | VAL | A | 364 | 10.338 | 31.821 | 67.570 | 1.00 | 33.68 | AAAA |
| ATOM | 2917 | CG1 | VAL | A | 364 | 11.739 | 31.722 | 68.162 | 1.00 | 34.13 | AAAA |
| ATOM | 2918 | CG2 | VAL | A | 364 | 10.337 | 32.715 | 66.347 | 1.00 | 31.83 | AAAA |
| ATOM | 2919 | C | VAL | A | 364 | 9.908 | 29.499 | 68.370 | 1.00 | 34.44 | AAAA |
| ATOM | 2920 | O | VAL | A | 364 | 10.789 | 28.640 | 68.430 | 1.00 | 36.01 | AAAA |
| ATOM | 2921 | N | LYS | A | 365 | 8.980 | 29.649 | 69.305 | 1.00 | 33.27 | AAAA |
| ATOM | 2922 | CA | LYS | A | 365 | 8.970 | 28.790 | 70.476 | 1.00 | 33.20 | AAAA |
| ATOM | 2923 | CB | LYS | A | 365 | 7.968 | 29.319 | 71.508 | 1.00 | 34.28 | AAAA |
| ATOM | 2924 | CG | LYS | A | 365 | 8.307 | 30.705 | 72.033 | 1.00 | 33.67 | AAAA |
| ATOM | 2925 | CD | LYS | A | 365 | 7.282 | 31.181 | 73.039 | 1.00 | 34.85 | AAAA |
| ATOM | 2926 | CE | LYS | A | 365 | 7.658 | 32.534 | 73.638 | 1.00 | 36.47 | AAAA |
| ATOM | 2927 | NZ | LYS | A | 365 | 6.698 | 32.990 | 74.710 | 1.00 | 37.91 | AAAA |
| ATOM | 2928 | C | LYS | A | 365 | 8.654 | 27.342 | 70.109 | 1.00 | 32.75 | AAAA |
| ATOM | 2929 | O | LYS | A | 365 | 9.071 | 26.421 | 70.818 | 1.00 | 31.95 | AAAA |
| ATOM | 2930 | N | ASP | A | 366 | 7.919 | 27.136 | 69.012 | 1.00 | 32.81 | AAAA |
| ATOM | 2931 | CA | ASP | A | 366 | 7.600 | 25.777 | 68.581 | 1.00 | 33.65 | AAAA |
| ATOM | 2932 | CB | ASP | A | 366 | 6.459 | 25.726 | 67.557 | 1.00 | 33.98 | AAAA |
| ATOM | 2933 | CG | ASP | A | 366 | 5.131 | 26.107 | 68.140 | 1.00 | 33.94 | AAAA |
| ATOM | 2934 | OD1 | ASP | A | 366 | 4.870 | 25.767 | 69.307 | 1.00 | 33.89 | AAAA |
| ATOM | 2935 | OD2 | ASP | A | 366 | 4.332 | 26.722 | 67.412 | 1.00 | 35.08 | AAAA |
| ATOM | 2936 | C | ASP | A | 366 | 8.820 | 25.167 | 67.940 | 1.00 | 33.05 | AAAA |
| ATOM | 2937 | O | ASP | A | 366 | 9.140 | 24.006 | 68.172 | 1.00 | 33.66 | AAAA |
| ATOM | 2938 | N | THR | A | 367 | 9.473 | 25.959 | 67.102 | 1.00 | 33.07 | AAAA |
| ATOM | 2939 | CA | THR | A | 367 | 10.684 | 25.540 | 66.412 | 1.00 | 32.27 | AAAA |
| ATOM | 2940 | CB | THR | A | 367 | 11.304 | 26.719 | 65.641 | 1.00 | 32.28 | AAAA |
| ATOM | 2941 | OG1 | THR | A | 367 | 10.473 | 27.039 | 64.520 | 1.00 | 30.64 | AAAA |
| ATOM | 2942 | CG2 | THR | A | 367 | 12.711 | 26.377 | 65.166 | 1.00 | 33.29 | AAAA |
| ATOM | 2943 | C | THR | A | 367 | 11.680 | 25.044 | 67.442 | 1.00 | 31.71 | AAAA |
| ATOM | 2944 | O | THR | A | 367 | 12.178 | 23.918 | 67.352 | 1.00 | 30.45 | AAAA |
| ATOM | 2945 | N | LEU | A | 368 | 11.955 | 25.896 | 68.426 | 1.00 | 32.05 | AAAA |
| ATOM | 2946 | CA | LEU | A | 368 | 12.888 | 25.560 | 69.482 | 1.00 | 32.49 | AAAA |
| ATOM | 2947 | CB | LEU | A | 368 | 13.085 | 26.749 | 70.421 | 1.00 | 32.27 | AAAA |
| ATOM | 2948 | CG | LEU | A | 368 | 14.097 | 27.809 | 69.960 | 1.00 | 32.71 | AAAA |
| ATOM | 2949 | CD1 | LEU | A | 368 | 15.488 | 27.170 | 69.899 | 1.00 | 33.00 | AAAA |
| ATOM | 2950 | CD2 | LEU | A | 368 | 13.709 | 28.393 | 68.597 | 1.00 | 31.86 | AAAA |
| ATOM | 2951 | C | LEU | A | 368 | 12.455 | 24.334 | 70.256 | 1.00 | 33.82 | AAAA |
| ATOM | 2952 | O | LEU | A | 368 | 13.266 | 23.133 | 70.489 | 1.00 | 34.29 | AAAA |
| ATOM | 2953 | N | GLU | A | 369 | 11.183 | 24.285 | 70.645 | 1.00 | 34.30 | AAAA |
| ATOM | 2954 | CA | GLU | A | 369 | 10.687 | 23.135 | 71.375 | 1.00 | 36.07 | AAAA |
| ATOM | 2955 | CB | GLU | A | 369 | 9.211 | 23.319 | 71.748 | 1.00 | 38.71 | AAAA |
| ATOM | 2956 | CG | GLU | A | 369 | 8.974 | 24.285 | 72.920 | 1.00 | 40.18 | AAAA |
| ATOM | 2957 | CD | GLU | A | 369 | 7.509 | 24.359 | 73.341 | 1.00 | 41.56 | AAAA |
| ATOM | 2958 | OE1 | GLU | A | 369 | 6.917 | 23.276 | 73.572 | 1.00 | 41.83 | AAAA |
| ATOM | 2959 | OE2 | GLU | A | 369 | 6.957 | 25.489 | 73.451 | 1.00 | 41.74 | AAAA |
| ATOM | 2960 | C | GLU | A | 369 | 10.893 | 21.822 | 70.611 | 1.00 | 37.16 | AAAA |
| ATOM | 2961 | O | GLU | A | 369 | 11.338 | 20.831 | 71.196 | 1.00 | 37.00 | AAAA |
| ATOM | 2962 | N | LYS | A | 370 | 10.586 | 21.788 | 69.315 | 1.00 | 37.71 | AAAA |
| ATOM | 2963 | CA | LYS | A | 370 | 10.797 | 20.547 | 68.567 | 1.00 | 38.46 | AAAA |
| ATOM | 2964 | CB | LYS | A | 370 | 10.166 | 20.604 | 67.177 | 1.00 | 39.96 | AAAA |
| ATOM | 2965 | CG | LYS | A | 370 | 8.646 | 20.532 | 67.186 | 1.00 | 42.68 | AAAA |
| ATOM | 2966 | CD | LYS | A | 370 | 8.092 | 20.320 | 65.775 | 1.00 | 44.54 | AAAA |
| ATOM | 2967 | CE | LYS | A | 370 | 6.572 | 20.075 | 65.781 | 1.00 | 45.55 | AAAA |
| ATOM | 2968 | NZ | LYS | A | 370 | 6.009 | 19.797 | 64.409 | 1.00 | 45.50 | AAAA |
| ATOM | 2969 | C | LYS | A | 370 | 12.282 | 20.235 | 68.452 | 1.00 | 38.34 | AAAA |
| ATOM | 2970 | O | LYS | A | 370 | 12.683 | 19.071 | 68.493 | 1.00 | 37.86 | AAAA |

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Figure 19-46

| | | | | | | | | | | | |
|--------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| ATOM | 2971 | N | ALA | A | 371 | 13.105 | 21.266 | 68.311 | 1.00 | 37.69 | AAAA |
| ATOM | 2972 | CA | ALA | A | 371 | 14.543 | 21.057 | 68.226 | 1.00 | 37.20 | AAAA |
| ATOM | 2973 | CB | ALA | A | 371 | 15.258 | 22.375 | 67.936 | 1.00 | 35.48 | AAAA |
| ATOM | 2974 | C | ALA | A | 371 | 15.023 | 20.477 | 69.558 | 1.00 | 37.63 | AAAA |
| ATOM | 2975 | O | ALA | A | 371 | 15.920 | 19.626 | 69.585 | 1.00 | 37.12 | AAAA |
| ATOM | 2976 | N | LYS | A | 372 | 14.426 | 20.930 | 70.665 | 1.00 | 37.59 | AAAA |
| ATOM | 2977 | CA | LYS | A | 372 | 14.796 | 20.432 | 71.995 | 1.00 | 37.46 | AAAA |
| ATOM | 2978 | CB | LYS | A | 372 | 14.022 | 21.156 | 73.095 | 1.00 | 36.52 | AAAA |
| ATOM | 2979 | CG | LYS | A | 372 | 14.287 | 22.634 | 73.111 | 1.00 | 22.67 | AAAA |
| ATOM | 2980 | CD | LYS | A | 372 | 13.309 | 23.396 | 74.022 | 1.00 | 22.67 | AAAA |
| ATOM | 2981 | CE | LYS | A | 372 | 13.600 | 24.874 | 73.901 | 1.00 | 22.67 | AAAA |
| ATOM | 2982 | NZ | LYS | A | 372 | 12.692 | 25.708 | 74.785 | 1.00 | 22.67 | AAAA |
| ATOM | 2983 | C | LYS | A | 372 | 14.495 | 18.957 | 72.077 | 1.00 | 37.60 | AAAA |
| ATOM | 2984 | O | LYS | A | 372 | 15.367 | 18.171 | 72.407 | 1.00 | 37.26 | AAAA |
| ATOM | 2985 | N | ALA | A | 373 | 13.249 | 18.595 | 71.789 | 1.00 | 38.17 | AAAA |
| ATOM | 2986 | CA | ALA | A | 373 | 12.812 | 17.206 | 71.829 | 1.00 | 39.55 | AAAA |
| ATOM | 2987 | CB | ALA | A | 373 | 11.365 | 17.109 | 71.395 | 1.00 | 39.34 | AAAA |
| ATOM | 2988 | C | ALA | A | 373 | 13.675 | 16.277 | 70.972 | 1.00 | 41.02 | AAAA |
| ATOM | 2989 | O | ALA | A | 373 | 14.366 | 15.410 | 71.561 | 1.00 | 42.26 | AAAA |
| ATOM | 2990 | OXT | ALA | A | 373 | 13.663 | 16.416 | 69.725 | 1.00 | 42.06 | AAAA |
| HETATM | 2991 | ZN | ZN | B | 951 | 23.696 | 34.788 | 54.072 | 1.00 | 27.38 | ZONE |
| HETATM | 2992 | O1 | SHA | C | 1 | 24.578 | 33.295 | 53.458 | 1.00 | 31.95 | SAHA |
| HETATM | 2993 | O2 | SHA | C | 1 | 24.294 | 35.218 | 51.444 | 1.00 | 33.51 | SAHA |
| HETATM | 2994 | N1 | SHA | C | 1 | 24.578 | 33.085 | 52.069 | 1.00 | 34.03 | SAHA |
| HETATM | 2995 | C1 | SHA | C | 1 | 24.063 | 34.053 | 51.246 | 1.00 | 34.25 | SAHA |
| HETATM | 2996 | C2 | SHA | C | 1 | 23.090 | 33.625 | 50.259 | 1.00 | 36.87 | SAHA |
| HETATM | 2997 | C3 | SHA | C | 1 | 23.548 | 33.781 | 48.816 | 1.00 | 39.33 | SAHA |
| HETATM | 2998 | C4 | SHA | C | 1 | 22.498 | 33.274 | 47.852 | 1.00 | 40.86 | SAHA |
| HETATM | 2999 | C5 | SHA | C | 1 | 21.590 | 34.413 | 47.455 | 1.00 | 43.37 | SAHA |
| HETATM | 3000 | C6 | SHA | C | 1 | 21.061 | 34.017 | 46.092 | 1.00 | 46.72 | SAHA |
| HETATM | 3001 | C7 | SHA | C | 1 | 19.754 | 34.714 | 45.787 | 1.00 | 48.75 | SAHA |
| HETATM | 3002 | C8 | SHA | C | 1 | 19.960 | 35.720 | 44.693 | 1.00 | 50.75 | SAHA |
| HETATM | 3003 | O3 | SHA | C | 1 | 20.381 | 35.467 | 43.575 | 1.00 | 51.08 | SAHA |
| HETATM | 3004 | N2 | SHA | C | 1 | 19.591 | 36.956 | 45.085 | 1.00 | 52.52 | SAHA |
| HETATM | 3005 | C9 | SHA | C | 1 | 19.842 | 38.330 | 44.507 | 1.00 | 54.25 | SAHA |
| HETATM | 3006 | C10 | SHA | C | 1 | 19.243 | 39.431 | 45.215 | 1.00 | 55.76 | SAHA |
| HETATM | 3007 | C11 | SHA | C | 1 | 19.423 | 40.804 | 44.727 | 1.00 | 56.53 | SAHA |
| HETATM | 3008 | C12 | SHA | C | 1 | 20.169 | 41.085 | 43.545 | 1.00 | 56.58 | SAHA |
| HETATM | 3009 | C13 | SHA | C | 1 | 20.755 | 39.942 | 42.827 | 1.00 | 55.93 | SAHA |
| HETATM | 3010 | C14 | SHA | C | 1 | 20.612 | 38.546 | 43.304 | 1.00 | 54.65 | SAHA |
| HETATM | 3011 | OH2 | WAT | D | 2 | 36.485 | 44.023 | 49.378 | 1.00 | 4.67 | SOLV |
| HETATM | 3012 | OH2 | WAT | D | 3 | 27.702 | 16.865 | 62.162 | 1.00 | 4.67 | SOLV |
| HETATM | 3013 | OH2 | WAT | D | 4 | 23.251 | 30.387 | 59.575 | 1.00 | 10.12 | SOLV |
| HETATM | 3014 | OH2 | WAT | D | 5 | 33.825 | 41.862 | 46.926 | 1.00 | 21.13 | SOLV |
| HETATM | 3015 | OH2 | WAT | D | 6 | 24.866 | 44.453 | 47.867 | 1.00 | 23.72 | SOLV |
| HETATM | 3016 | OH2 | WAT | D | 7 | 34.145 | 20.442 | 33.590 | 1.00 | 18.19 | SOLV |
| HETATM | 3017 | OH2 | WAT | D | 8 | 7.921 | 29.753 | 62.099 | 1.00 | 20.79 | SOLV |
| HETATM | 3018 | OH2 | WAT | D | 9 | 17.863 | 6.978 | 64.018 | 1.00 | 28.94 | SOLV |
| HETATM | 3019 | OH2 | WAT | D | 10 | 35.580 | 44.610 | 74.823 | 1.00 | 31.62 | SOLV |
| HETATM | 3020 | OH2 | WAT | D | 11 | 49.208 | 27.797 | 65.303 | 1.00 | 14.70 | SOLV |
| HETATM | 3021 | OH2 | WAT | D | 12 | 20.490 | 34.049 | 61.067 | 1.00 | 25.01 | SOLV |
| HETATM | 3022 | OH2 | WAT | D | 13 | 44.757 | 33.106 | 46.084 | 1.00 | 25.90 | SOLV |
| HETATM | 3023 | OH2 | WAT | D | 14 | 22.457 | 60.823 | 57.444 | 1.00 | 15.21 | SOLV |
| HETATM | 3024 | OH2 | WAT | D | 15 | 3.399 | 32.742 | 65.163 | 1.00 | 20.66 | SOLV |
| HETATM | 3025 | OH2 | WAT | D | 16 | 32.273 | 51.414 | 45.610 | 1.00 | 22.37 | SOLV |
| HETATM | 3026 | OH2 | WAT | D | 17 | 26.328 | 42.873 | 73.427 | 1.00 | 27.86 | SOLV |
| HETATM | 3027 | OH2 | WAT | D | 18 | 48.249 | 24.121 | 56.778 | 1.00 | 15.09 | SOLV |
| HETATM | 3028 | OH2 | WAT | D | 19 | 15.249 | 44.552 | 72.082 | 1.00 | 40.95 | SOLV |
| HETATM | 3029 | OH2 | WAT | D | 20 | 26.444 | 9.269 | 52.633 | 1.00 | 26.66 | SOLV |
| HETATM | 3030 | OH2 | WAT | D | 21 | 26.554 | 18.383 | 59.650 | 1.00 | 11.42 | SOLV |
| HETATM | 3031 | OH2 | WAT | D | 22 | 39.456 | 25.964 | 72.316 | 1.00 | 20.32 | SOLV |
| HETATM | 3032 | OH2 | WAT | D | 23 | 26.743 | 37.600 | 38.359 | 1.00 | 37.22 | SOLV |
| HETATM | 3033 | OH2 | WAT | D | 24 | 44.666 | 23.818 | 39.068 | 1.00 | 32.27 | SOLV |
| HETATM | 3034 | OH2 | WAT | D | 25 | 14.714 | 52.213 | 70.663 | 1.00 | 29.24 | SOLV |
| HETATM | 3035 | OH2 | WAT | D | 26 | 45.129 | 18.856 | 69.864 | 1.00 | 29.58 | SOLV |
| HETATM | 3036 | OH2 | WAT | D | 27 | 30.024 | 17.886 | 49.758 | 1.00 | 15.52 | SOLV |

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Figure 19-47

| | | | | | | | | | | |
|-------------|-----|-----|---|----|--------|--------|--------|------|-------|------|
| HETATM 3037 | OH2 | WAT | D | 28 | 20.659 | 28.788 | 43.520 | 1.00 | 28.55 | SOLV |
| HETATM 3038 | OH2 | WAT | D | 29 | 32.271 | 38.000 | 53.512 | 1.00 | 47.72 | SOLV |
| HETATM 3039 | OH2 | WAT | D | 30 | 18.285 | 29.333 | 54.536 | 1.00 | 21.34 | SOLV |
| HETATM 3040 | OH2 | WAT | D | 31 | 49.978 | 38.669 | 73.461 | 1.00 | 31.02 | SOLV |
| HETATM 3041 | OH2 | WAT | D | 32 | 21.587 | 50.386 | 71.043 | 1.00 | 14.52 | SOLV |
| HETATM 3042 | OH2 | WAT | D | 33 | 46.784 | 32.121 | 33.375 | 1.00 | 31.79 | SOLV |
| HETATM 3043 | OH2 | WAT | D | 34 | 33.359 | 39.755 | 49.117 | 1.00 | 16.13 | SOLV |
| HETATM 3044 | OH2 | WAT | D | 35 | 7.687 | 37.657 | 51.568 | 1.00 | 27.22 | SOLV |
| HETATM 3045 | OH2 | WAT | D | 36 | 44.238 | 35.392 | 33.961 | 1.00 | 19.67 | SOLV |
| HETATM 3046 | OH2 | WAT | D | 37 | 10.908 | 25.384 | 58.206 | 1.00 | 33.51 | SOLV |
| HETATM 3047 | OH2 | WAT | D | 38 | 36.758 | 27.243 | 70.552 | 1.00 | 39.61 | SOLV |
| HETATM 3048 | OH2 | WAT | D | 39 | 45.825 | 46.691 | 54.654 | 1.00 | 32.43 | SOLV |
| HETATM 3049 | OH2 | WAT | D | 40 | 52.489 | 20.282 | 52.165 | 1.00 | 39.37 | SOLV |
| HETATM 3050 | OH2 | WAT | D | 42 | 12.117 | 17.831 | 56.596 | 1.00 | 27.74 | SOLV |
| HETATM 3051 | OH2 | WAT | D | 43 | 45.023 | 26.168 | 35.172 | 1.00 | 14.09 | SOLV |
| HETATM 3052 | OH2 | WAT | D | 44 | 39.392 | 12.771 | 62.066 | 1.00 | 35.15 | SOLV |
| HETATM 3053 | OH2 | WAT | D | 45 | 3.930 | 26.970 | 63.814 | 1.00 | 22.23 | SOLV |
| HETATM 3054 | OH2 | WAT | D | 46 | 8.454 | 19.321 | 71.677 | 1.00 | 32.36 | SOLV |
| HETATM 3055 | OH2 | WAT | D | 47 | 20.280 | 18.126 | 73.237 | 1.00 | 33.88 | SOLV |
| HETATM 3056 | OH2 | WAT | D | 48 | 9.321 | 39.409 | 54.873 | 1.00 | 18.57 | SOLV |
| HETATM 3057 | OH2 | WAT | D | 49 | 50.852 | 41.323 | 58.048 | 1.00 | 21.25 | SOLV |
| HETATM 3058 | OH2 | WAT | D | 50 | 37.134 | 34.599 | 60.315 | 1.00 | 61.70 | SOLV |
| HETATM 3059 | OH2 | WAT | D | 51 | 14.944 | 62.815 | 48.613 | 1.00 | 42.50 | SOLV |
| HETATM 3060 | OH2 | WAT | D | 52 | 6.494 | 33.164 | 51.420 | 1.00 | 40.65 | SOLV |
| HETATM 3061 | OH2 | WAT | D | 53 | 24.913 | 44.799 | 72.298 | 1.00 | 17.10 | SOLV |
| HETATM 3062 | OH2 | WAT | D | 54 | 51.156 | 35.095 | 48.814 | 1.00 | 23.05 | SOLV |
| HETATM 3063 | OH2 | WAT | D | 55 | 16.518 | 41.750 | 45.596 | 1.00 | 49.25 | SOLV |
| HETATM 3064 | OH2 | WAT | D | 56 | 10.326 | 16.413 | 61.267 | 1.00 | 46.03 | SOLV |
| HETATM 3065 | OH2 | WAT | D | 57 | 25.316 | 47.708 | 73.062 | 1.00 | 22.73 | SOLV |
| HETATM 3066 | OH2 | WAT | D | 58 | 4.013 | 33.865 | 76.173 | 1.00 | 44.82 | SOLV |
| HETATM 3067 | OH2 | WAT | D | 59 | 24.846 | 18.072 | 36.805 | 1.00 | 34.67 | SOLV |
| HETATM 3068 | OH2 | WAT | D | 60 | 15.930 | 56.853 | 61.737 | 1.00 | 55.56 | SOLV |
| HETATM 3069 | OH2 | WAT | D | 61 | 49.662 | 44.249 | 48.982 | 1.00 | 28.72 | SOLV |
| HETATM 3070 | OH2 | WAT | D | 62 | 23.232 | 17.421 | 53.920 | 1.00 | 13.11 | SOLV |
| HETATM 3071 | OH2 | WAT | D | 63 | 39.293 | 23.035 | 33.289 | 1.00 | 35.79 | SOLV |
| HETATM 3072 | OH2 | WAT | D | 64 | 19.908 | 20.169 | 44.339 | 1.00 | 24.33 | SOLV |
| HETATM 3073 | OH2 | WAT | D | 65 | 33.259 | 21.655 | 69.560 | 1.00 | 45.10 | SOLV |
| HETATM 3074 | OH2 | WAT | D | 66 | 27.528 | 53.947 | 68.629 | 1.00 | 44.79 | SOLV |
| HETATM 3075 | OH2 | WAT | D | 67 | 18.774 | 48.716 | 52.865 | 1.00 | 54.01 | SOLV |
| HETATM 3076 | OH2 | WAT | D | 68 | 10.877 | 29.062 | 63.401 | 1.00 | 27.08 | SOLV |
| HETATM 3077 | OH2 | WAT | D | 69 | 43.057 | 31.367 | 28.786 | 1.00 | 30.16 | SOLV |
| HETATM 3078 | OH2 | WAT | D | 70 | 24.816 | 44.057 | 43.447 | 1.00 | 20.11 | SOLV |
| HETATM 3079 | OH2 | WAT | D | 71 | 37.368 | 38.823 | 46.381 | 1.00 | 33.55 | SOLV |
| HETATM 3080 | OH2 | WAT | D | 72 | 9.038 | 18.327 | 63.519 | 1.00 | 31.34 | SOLV |
| HETATM 3081 | OH2 | WAT | D | 73 | 51.799 | 20.829 | 65.265 | 1.00 | 28.32 | SOLV |
| HETATM 3082 | OH2 | WAT | D | 74 | 17.556 | 58.515 | 57.254 | 1.00 | 19.27 | SOLV |
| HETATM 3083 | OH2 | WAT | D | 75 | 28.436 | 27.904 | 79.425 | 1.00 | 27.13 | SOLV |
| HETATM 3084 | OH2 | WAT | D | 76 | 18.939 | 35.798 | 35.800 | 1.00 | 94.18 | SOLV |
| HETATM 3085 | OH2 | WAT | D | 77 | 34.359 | 31.251 | 46.688 | 1.00 | 73.70 | SOLV |
| HETATM 3086 | OH2 | WAT | D | 78 | 44.373 | 51.649 | 60.029 | 1.00 | 30.23 | SOLV |
| HETATM 3087 | OH2 | WAT | D | 79 | 28.537 | 63.478 | 48.324 | 1.00 | 21.09 | SOLV |
| HETATM 3088 | OH2 | WAT | D | 80 | 6.869 | 44.113 | 72.030 | 1.00 | 28.59 | SOLV |
| HETATM 3089 | OH2 | WAT | D | 81 | 42.882 | 18.761 | 71.115 | 1.00 | 31.80 | SOLV |
| HETATM 3090 | OH2 | WAT | D | 82 | 36.712 | 59.078 | 53.901 | 1.00 | 40.11 | SOLV |
| HETATM 3091 | OH2 | WAT | D | 83 | 37.506 | 42.495 | 40.104 | 1.00 | 51.37 | SOLV |
| HETATM 3092 | OH2 | WAT | D | 84 | 40.054 | 38.439 | 55.415 | 1.00 | 20.07 | SOLV |
| HETATM 3093 | OH2 | WAT | D | 85 | 32.170 | 56.633 | 72.920 | 1.00 | 45.23 | SOLV |
| HETATM 3094 | OH2 | WAT | D | 86 | 24.470 | 53.877 | 47.119 | 1.00 | 41.18 | SOLV |
| HETATM 3095 | OH2 | WAT | D | 87 | 48.585 | 35.663 | 67.518 | 1.00 | 33.40 | SOLV |
| HETATM 3096 | OH2 | WAT | D | 88 | 29.541 | 57.166 | 42.788 | 1.00 | 44.61 | SOLV |
| HETATM 3097 | OH2 | WAT | D | 89 | 47.814 | 28.707 | 41.228 | 1.00 | 45.64 | SOLV |
| HETATM 3098 | OH2 | WAT | D | 90 | 49.377 | 52.112 | 63.320 | 1.00 | 22.26 | SOLV |
| HETATM 3099 | OH2 | WAT | D | 91 | 44.219 | 43.589 | 43.912 | 1.00 | 39.90 | SOLV |
| HETATM 3100 | OH2 | WAT | D | 92 | 25.913 | 61.639 | 75.382 | 1.00 | 48.28 | SOLV |
| HETATM 3101 | OH2 | WAT | D | 93 | 8.623 | 30.749 | 49.707 | 1.00 | 40.37 | SOLV |
| HETATM 3102 | OH2 | WAT | D | 94 | 45.634 | 41.080 | 40.990 | 1.00 | 21.46 | SOLV |

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Figure 19-48

| | | | | | | | | | | | |
|--------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|
| HETATM | 3103 | OH2 | WAT | D | 95 | 29.984 | 34.886 | 51.725 | 1.00 | 35.75 | SOLV |
| HETATM | 3104 | OH2 | WAT | D | 96 | 13.051 | 21.934 | 49.804 | 1.00 | 46.73 | SOLV |
| HETATM | 3105 | OH2 | WAT | D | 97 | 32.412 | 65.913 | 55.822 | 1.00 | 43.39 | SOLV |
| HETATM | 3106 | OH2 | WAT | D | 98 | 35.056 | 43.390 | 38.348 | 1.00 | 34.53 | SOLV |
| HETATM | 3107 | OH2 | WAT | D | 99 | 22.360 | 47.680 | 60.688 | 1.00 | 19.16 | SOLV |
| HETATM | 3108 | OH2 | WAT | D | 100 | 50.755 | 19.722 | 57.906 | 1.00 | 42.45 | SOLV |
| HETATM | 3109 | OH2 | WAT | D | 101 | 7.875 | 37.690 | 74.094 | 1.00 | 37.18 | SOLV |
| HETATM | 3110 | OH2 | WAT | D | 102 | 24.080 | 26.796 | 43.617 | 1.00 | 30.72 | SOLV |
| HETATM | 3111 | OH2 | WAT | D | 103 | 45.206 | 34.126 | 75.765 | 1.00 | 39.89 | SOLV |
| HETATM | 3112 | OH2 | WAT | D | 104 | 26.110 | 54.786 | 40.685 | 1.00 | 29.58 | SOLV |
| HETATM | 3113 | OH2 | WAT | D | 105 | 25.918 | 39.658 | 77.647 | 1.00 | 44.04 | SOLV |
| HETATM | 3114 | OH2 | WAT | D | 106 | 41.578 | 18.191 | 36.809 | 1.00 | 42.22 | SOLV |
| HETATM | 3115 | OH2 | WAT | D | 107 | 31.945 | 51.420 | 73.896 | 1.00 | 41.15 | SOLV |
| HETATM | 3116 | OH2 | WAT | D | 108 | 16.722 | 60.311 | 51.182 | 1.00 | 48.74 | SOLV |
| HETATM | 3117 | OH2 | WAT | D | 109 | 43.604 | 38.573 | 78.141 | 1.00 | 36.22 | SOLV |
| HETATM | 3118 | OH2 | WAT | D | 110 | 16.063 | 15.496 | 69.430 | 1.00 | 55.36 | SOLV |
| HETATM | 3119 | OH2 | WAT | D | 111 | 21.630 | 22.785 | 49.145 | 1.00 | 36.52 | SOLV |
| HETATM | 3120 | OH2 | WAT | D | 112 | 27.479 | 56.647 | 44.026 | 1.00 | 50.82 | SOLV |
| HETATM | 3121 | OH2 | WAT | D | 113 | 14.739 | 51.674 | 61.674 | 1.00 | 35.55 | SOLV |
| HETATM | 3122 | OH2 | WAT | D | 114 | 50.063 | 26.435 | 54.358 | 1.00 | 50.86 | SOLV |
| HETATM | 3123 | OH2 | WAT | D | 115 | 43.935 | 38.427 | 73.129 | 1.00 | 44.21 | SOLV |
| HETATM | 3124 | OH2 | WAT | D | 116 | 49.707 | 31.478 | 57.709 | 1.00 | 36.11 | SOLV |
| HETATM | 3125 | OH2 | WAT | D | 117 | 25.032 | 43.463 | 55.676 | 1.00 | 38.06 | SOLV |
| HETATM | 3126 | OH2 | WAT | D | 118 | 10.618 | 46.623 | 59.838 | 1.00 | 26.33 | SOLV |
| HETATM | 3127 | OH2 | WAT | D | 119 | 48.466 | 33.382 | 61.437 | 1.00 | 19.82 | SOLV |
| HETATM | 3128 | OH2 | WAT | D | 120 | 44.157 | 40.058 | 37.907 | 1.00 | 42.95 | SOLV |
| HETATM | 3129 | OH2 | WAT | D | 121 | 51.267 | 29.446 | 52.889 | 1.00 | 38.93 | SOLV |
| HETATM | 3130 | OH2 | WAT | D | 122 | 16.653 | 15.228 | 72.975 | 1.00 | 45.41 | SOLV |
| HETATM | 3131 | OH2 | WAT | D | 123 | 36.898 | 45.148 | 41.936 | 1.00 | 27.00 | SOLV |
| HETATM | 3132 | OH2 | WAT | D | 124 | 49.655 | 34.591 | 59.117 | 1.00 | 38.97 | SOLV |
| HETATM | 3133 | OH2 | WAT | D | 125 | 12.285 | 57.594 | 42.107 | 1.00 | 23.56 | SOLV |
| HETATM | 3134 | OH2 | WAT | D | 126 | 28.294 | 57.644 | 73.289 | 1.00 | 34.79 | SOLV |
| HETATM | 3135 | OH2 | WAT | D | 127 | 19.138 | 60.403 | 61.551 | 1.00 | 28.58 | SOLV |
| HETATM | 3136 | OH2 | WAT | D | 128 | 30.300 | 33.685 | 34.047 | 1.00 | 27.37 | SOLV |
| HETATM | 3137 | OH2 | WAT | D | 129 | 40.898 | 53.983 | 47.254 | 1.00 | 16.30 | SOLV |
| HETATM | 3138 | OH2 | WAT | D | 130 | 43.550 | 32.160 | 38.272 | 1.00 | 38.86 | SOLV |
| HETATM | 3139 | OH2 | WAT | D | 131 | 18.624 | 13.959 | 56.194 | 1.00 | 37.70 | SOLV |
| HETATM | 3140 | OH2 | WAT | D | 132 | 18.580 | 12.901 | 62.894 | 1.00 | 27.28 | SOLV |
| HETATM | 3141 | OH2 | WAT | D | 133 | 35.830 | 30.296 | 50.621 | 1.00 | 42.47 | SOLV |
| HETATM | 3142 | OH2 | WAT | D | 134 | 51.219 | 35.855 | 51.878 | 1.00 | 20.37 | SOLV |
| HETATM | 3143 | OH2 | WAT | D | 135 | 50.428 | 22.486 | 49.267 | 1.00 | 39.37 | SOLV |
| HETATM | 3144 | OH2 | WAT | D | 136 | 51.633 | 29.369 | 63.918 | 1.00 | 33.99 | SOLV |
| HETATM | 3145 | OH2 | WAT | D | 137 | 46.384 | 43.924 | 55.825 | 1.00 | 22.63 | SOLV |
| HETATM | 3146 | OH2 | WAT | D | 138 | 30.356 | 25.767 | 28.762 | 1.00 | 25.84 | SOLV |
| HETATM | 3147 | OH2 | WAT | D | 139 | 25.070 | 47.842 | 60.819 | 1.00 | 25.00 | SOLV |
| HETATM | 3148 | OH2 | WAT | D | 140 | 47.097 | 49.394 | 69.367 | 1.00 | 30.58 | SOLV |
| HETATM | 3149 | OH2 | WAT | D | 141 | 15.246 | 37.581 | 73.398 | 1.00 | 36.82 | SOLV |
| HETATM | 3150 | OH2 | WAT | D | 142 | 8.341 | 23.099 | 64.695 | 1.00 | 35.89 | SOLV |
| HETATM | 3151 | OH2 | WAT | D | 143 | 30.065 | 18.220 | 46.048 | 1.00 | 14.26 | SOLV |
| HETATM | 3152 | OH2 | WAT | D | 144 | 11.930 | 46.453 | 57.606 | 1.00 | 36.15 | SOLV |

INTERNATIONAL SEARCH REPORT

International application No.

PCT/US00/24700

| A. CLASSIFICATION OF SUBJECT MATTER IPC(7) :Co7K 14/00; G01N 33/573 US CL :Please See Extra Sheet. According to International Patent Classification (IPC) or to both national classification and IPC | | |
|---|--|--|
| B. FIELDS SEARCHED Minimum documentation searched (classification system followed by classification symbols) U.S. : Please See Extra Sheet. Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) Please See Extra Sheet. | | |
| C. DOCUMENTS CONSIDERED TO BE RELEVANT | | |
| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
| Y | KAKUTA et al. Crystal Structure of the Sulfotransferase Domain of Human Heparan Sulfate N-Deacetylase/N-Sulfotransferase 1. The Journal of Biological Chemistry. 16 April 1999, Volume 274, Number 16, pages 10673-10676, see especially the abstract. | 1-19 |
| Y | SUEYOSHI et al. A role of Lys-614 in the sulfotransferase activity of human heparan sulfate N-deacetylase/N-sulfotransferase. FEBS Letters. 1998, Volume 433, pages 211-214, see especially the abstract. | 1-19 |
| <input checked="" type="checkbox"/> Further documents are listed in the continuation of Box C. <input type="checkbox"/> See patent family annex. | | |
| * Special categories of cited documents: "A" document defining the general state of the art which is not considered to be of particular relevance "E" earlier document published on or after the international filing date "I" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) "O" document referring to an oral disclosure, use, exhibition or other means "P" document published prior to the international filing date but later than the priority date claimed | "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention "X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art "Z" document member of the same patent family | |
| Date of the actual completion of the international search | | Date of mailing of the international search report |
| 29 DECEMBER 2000 | | 25 JAN 2001 |
| Name and mailing address of the ISA/US Commissioner of Patents and Trademarks Box PCT Washington, D.C. 20231 Facsimile No. (703) 305-3230 | | Authorized officer <i>Ardin Marschel</i> ARDIN MARSCHEL Telephone No. (703) 308-0196 |

INTERNATIONAL SEARCH REPORT

International application No.

PCT/US00/24700

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|-----------|---|-----------------------|
| Y | AHMAD et al. WD Repeats of the p48 Subunit of Chicken Chromatin Assembly Factor-1 Required for in Vitro Interaction with Chicken Histone Deacetylase-2. The Journal of Biological Chemistry. 04 June 1999, Volume 274, Number 23, pages 16646-16653, see especially the abstract. | 1-19 |
| Y | JOHN et al. Rhizobium NodB protein involved in nodulation signal synthesis is a chitooligosaccharide deacetylase. Proceedings of the National Academy of Sciences, USA. January 1993, Volume 90, pages 625-629, see especially the abstract. | 1-19 |
| A | US 5,780,594 A (CARTER) 14 July 1998, see the entire disclosure. | 1-19 |

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US00/24700

A. CLASSIFICATION OF SUBJECT MATTER:

US CL :

530/350 and 435/7.2

B. FIELDS SEARCHED

Minimum documentation searched

Classification System: U.S.

530/300,333,350; 435/6,7,2; 514/2

B. FIELDS SEARCHED

Electronic data bases consulted (Name of data base and where practicable terms used):

CAS, BIOTECH ABS, MEDLINE, EMBASE, WPI, WEST covering search terms: deacetylase, human, crystal, histone, inhibitor, x-ray, and crystallography

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